



STIC Search Report

Biotech-Chem Library

STIC Database Tracking Number: 111586

TO: Michael Lavilla
Location: REM 5e79
Thursday, January 08, 2004
Art Unit: 1775
Phone: 571-272-1539
Serial Number: 09 / 700821

From: Jan Delaval
Location: Biotech-Chem Library
Remsen Building – 1A51
Phone: 571-272-2504
jan.delaval@uspto.gov

Search Notes

10/6/2000

U

=> fil reg
FILE 'REGISTRY' ENTERED AT 07:55:34 ON 08 JAN 2004
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STRUCTURE FILE UPDATES: 6 JAN 2004 HIGHEST RN 634878-43-6
DICTIONARY FILE UPDATES: 6 JAN 2004 HIGHEST RN 634878-43-6

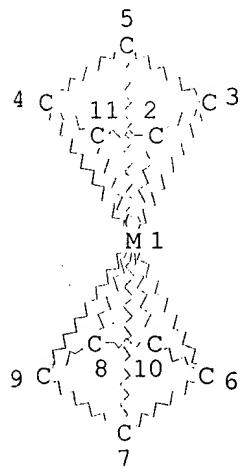
TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> d sta que 116
L7 STR



NODE ATTRIBUTES:

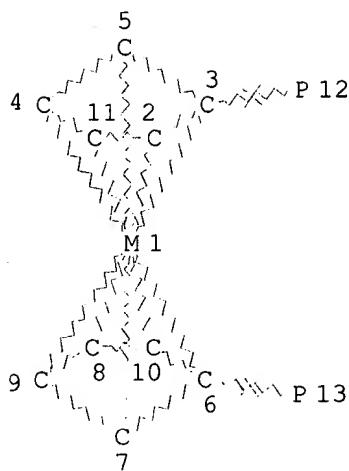
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 11

STEREO ATTRIBUTES: NONE

L9 SCR 2017
L11 7674 SEA FILE=REGISTRY SSS FUL L7 AND L9
L12 423 SÉA FILE=REGISTRY ABB=ON PLU=ON L11 AND (FE AND RH)/ELS
L13 STR



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 13

STEREO ATTRIBUTES: NONE

L15 3743 SEA FILE=REGISTRY SUB=L11 SSS FUL L13
 L16 265 SEA FILE=REGISTRY ABB=ON PLU=ON L12 AND L15

=> d his

(FILE 'HOME' ENTERED AT 07:07:27 ON 08 JAN 2004)
 SET COST OFF

FILE 'HCAPLUS' ENTERED AT 07:07:47 ON 08 JAN 2004
 L1 1 S (WO2000-GB3851 OR GB99-23952)/AP, PRN
 E BURK M/AU
 L2 127 S E3, E5, E11-E13
 E GERLACH A/AU
 L3 50 S E3, E4, E21
 E CHIROTECH/PA, CS
 L4 213 S E3-E31
 SEL RN L1

FILE 'REGISTRY' ENTERED AT 07:10:11 ON 08 JAN 2004
 L5 9 S E1-E9
 E FERROCENE/CN
 L6 1 S E3
 L7 STR
 L8 50 S L7
 L9 SCR 2017
 L10 50 S L7 AND L9
 L11 7674 S L7 AND L9 FUL
 SAV L11 LAVILLA700/A
 L12 423 S L11 AND (FE AND RH)/ELS
 L13 STR L7
 L14 50 S L13 SAM SUB=L11
 L15 3743 S L13 FUL SUB=L11
 SAV L15 LAVILLA700A/A
 L16 265 S L12 AND L15

L17 STR L13
 L18 3 S L17 SAM SUB=L15
 L19 142 S L17 FUL SUB=L15
 SAV L19 LAVILLA700B/A
 L20 26 S L16 AND L19
 L21 20 S L20 AND 1/RH
 L22 16 S L21 AND 2/P AND 1/FE
 L23 4 S L21 NOT L22
 L24 15 S L22 NOT C27H37F6FEO2P2RH

FILE 'HCAOLD' ENTERED AT 07:20:25 ON 08 JAN 2004
 L25 0 S L24

FILE 'USPATFULL, USPAT2' ENTERED AT 07:20:29 ON 08 JAN 2004
 L26 0 S L24

FILE 'HCAPLUS' ENTERED AT 07:20:33 ON 08 JAN 2004
 L27 15 S L24
 L28 5 S L27 AND L1-L4
 E ALDEHYDE/CT
 L29 386960 S E17+NT
 L30 48009 S E3-E67
 L31 502889 S ?ALDEHYD?
 L32 1876 S L15
 E HYDROGENATION/CT
 L33 46596 S E3+NT
 L34 36933 S E20+NT
 L35 132 S E32+NT
 L36 1397 S E36+NT
 L37 104 S L16
 L38 22 S L37 AND L29-L31
 L39 7 S L38 AND L33-L36
 L40 8 S L38 AND ?ALCOHOL?
 L41 4 S L39 AND L40
 L42 11 S L28, L39-L41
 L43 1 S L27 AND P/DT
 L44 21 S L27, L42, L43
 L45 17 S L44 AND ?HYDROGENAT?
 L46 9 S L45 AND L29-L31
 L47 9 S L28, L46
 L48 12 S L44, L45 NOT L47
 SEL HIT RN L48

FILE 'REGISTRY' ENTERED AT 07:35:33 ON 08 JAN 2004
 L49 13 S E1-E13
 L50 10 S L49 AND L11

FILE 'HCAPLUS' ENTERED AT 07:36:42 ON 08 JAN 2004
 L51 18 S L50
 L52 15 S L51 AND (PY<=1999 OR PRY<=1999 OR AY<=1999)
 L53 4 S L47 AND (PY<=1999 OR PRY<=1999 OR AY<=1999)
 L54 19 S L28, L52, L53
 L55 19 S L54 AND L1-L4, L27-L48, L51-L54
 L56 4071 S PHOSPHOTUNGSTIC ACID
 L57 2345 S PHOSPHOMOLYBDIC ACID
 L58 1136 S SILICOTUNGSTIC ACID

FILE 'REGISTRY' ENTERED AT 07:39:46 ON 08 JAN 2004
 L59 3 S 1343-93-7 OR 12026-57-2 OR 12027-38-2
 L60 3 S 12534-77-9 OR 12379-13-4 OR 12363-31-4
 L61 1638 S (12534-77-9 OR 12379-13-4 OR 12363-31-4) /CRN

FILE 'HCAPLUS' ENTERED AT 07:41:13 ON 08 JAN 2004

L62 3445 S L59 OR L60
 L63 4365 S L61
 L64 3 S L56-L58, L62-L63 AND L37
 L65 2 S L16 AND ALUMINA

FILE 'REGISTRY' ENTERED AT 07:42:26 ON 08 JAN 2004
 L66 1 S 1344-28-1

FILE 'HCAPLUS' ENTERED AT 07:42:40 ON 08 JAN 2004
 L67 218225 S L66
 L68 342015 S AL2O3 OR ALUMINUM OXIDE
 L69 2 S L67, L68 AND L16
 L70 0 S TETRAFLUOROETHYLENE PERFLUORO VINYL ETHER SULFONATE
 L71 0 S TETRAFLUOROETHYLENE PERFLUORO VINYL ETHER SULPHONATE
 L72 0 S TETRAFLUOROETHYLENE PERFLUOROVINYL ETHER SULPHONATE
 L73 0 S TETRAFLUOROETHYLENE PERFLUOROVINYL ETHER SULFONATE
 L74 0 S ?TETRAFLUOROETHYLENE? AND L16
 L75 6 S ?VINYL? AND L16
 L76 163 S ?TETRAFLUOROETHYLEN? (L) ?VINYL? (L) (?SULFONATE? OR ?SULPHON
 L77 23774 S PTFE
 L78 60 S L77 (L) ?VINYL? (L) (?SULFONATE? OR ?SULPHONATE?)

FILE 'REGISTRY' ENTERED AT 07:47:13 ON 08 JAN 2004
 L79 1 S 9002-84-0
 L80 1 S 116-14-3
 L81 3998 S 116-14-3/CRN
 L82 412 S L81 AND S/ELS
 L83 76 S L82 AND NR>=1
 L84 336 S L82 NOT L83
 L85 247 S L84 NOT N/ELS
 L86 97 S L85 AND 2/NC
 L87 127 S L85 AND 3/NC
 L88 23 S L85 NOT L86, L87
 L89 244 S L85 NOT SI/ELS

FILE 'HCAPLUS' ENTERED AT 07:52:06 ON 08 JAN 2004
 L90 0 S L89 AND L16
 L91 0 S L79, L80 AND L16
 L92 0 S L82 AND L16
 L93 19 S L64, L65, L69, L55

FILE 'REGISTRY' ENTERED AT 07:53:24 ON 08 JAN 2004
 FILE 'HCAPLUS' ENTERED AT 07:53:31 ON 08 JAN 2004
 L94 19 S L93 AND (RH OR ?RHODIUM?)

FILE 'REGISTRY' ENTERED AT 07:55:34 ON 08 JAN 2004

FILE 'HCAPLUS' ENTERED AT 07:55:42 ON 08 JAN 2004
 SEL HIT RN L94

FILE 'REGISTRY' ENTERED AT 07:57:38 ON 08 JAN 2004
 L95 59 S E14-E72
 L96 31 S L16 AND L95
 L97 28 S L95 NOT L96
 L98 12 S L97 AND L11
 L99 16 S L97 NOT L98

FILE 'HCAPLUS' ENTERED AT 07:59:28 ON 08 JAN 2004
 L100 26 S L96
 L101 20 S L100 AND (PY<=1999 OR PRY<=1999 OR AY<=1999)
 L102 16 S L101 AND L94
 L103 4 S L101 NOT L102

L104 20 S L101-L103

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=> fil hcaplus
FILE 'HCAPLUS' ENTERED AT 08:01:16 ON 08 JAN 2004
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FILE COVERS 1907 - 8 Jan 2004 VOL 140 ISS 2
FILE LAST UPDATED: 6 Jan 2004 (20040106/ED)

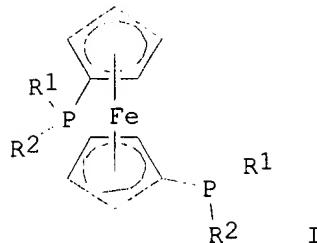
This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d 1104 all hitstr tot

L104 ANSWER 1 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2001:283853 HCAPLUS
DN 134:312797
ED Entered STN: 20 Apr 2001
TI Supported ferrocene-based catalysts for selective aldehyde hydrogenation
IN Burk, Mark Joseph; Gerlach, Arne
PA Chirotech Technology Limited, UK
SO PCT Int. Appl., 15 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM B01J031-22
 ICS B01J031-28; C07C045-62
CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)
 Section cross-reference(s): 23, 67

FAN.CNT	1	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001026807	A1	20010419	WO 2000-GB3851	20001006	<--
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM					
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG					
EP	1222026	A1	20020717	EP 2000-964538	20001006	<--
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL					
JP	2003511229	T2	20030325	JP 2001-529860	20001006	<--
PRAI	GB 1999-23952	A	19991008			<--
	WO 2000-GB3851	W	20001006			<--

OS MARPAT 134:312797
 GI



AB A supported catalyst comprises a cationic **rhodium** (I) complex of formula I, wherein R1 and R2 are the same or different C_{≤30} hydrocarbyl groups, or R1 and R2 are linked to form a ring, and a heterogeneous support medium that provides anionic binding sites. Such a complex is particularly useful as a catalyst in a process of **hydrogenating an aldehyde** to produce the corresponding **primary alc.** Stirring 288 mg **phosphotungstic acid** with 4 g silica gel for 1 h, stirring the mixture with 64 mg [(DiPFc)Rh(COD)]BF₄ (COD = cyclooctadiene; DiPFc 1,1'-bis(disopropylphosphino)ferrocene) gave a catalyst, which reduced pentanal to pentanol in 100% yield.

ST supported ferrocene catalyst selective **aldehyde hydrogenation**; pentanal **hydrogenation catalyst** **rhodium ferrocene complex**

IT Metallocenes
 RL: CAT (Catalyst use); USES (Uses)
 (ferrocenes; supported ferrocene-based catalysts for selective **aldehyde hydrogenation**)

IT **Alcohols, preparation**
 RL: IMF (Industrial manufacture); PREP (Preparation)
 (primary; supported ferrocene-based catalysts for selective **aldehyde hydrogenation**)

IT **Hydrogenation catalysts**
 (supported ferrocene-based catalysts for selective **aldehyde hydrogenation**)

IT **Aldehydes, reactions**
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (supported ferrocene-based catalysts for selective **aldehyde hydrogenation**)

IT 255064-36-9
 RL: CAT (Catalyst use); USES (Uses)
 (supported ferrocene-based catalysts for selective **aldehyde hydrogenation**)

IT 7440-16-6DP, **Rhodium**, complex with 1,1'-bis(disopropylphosphino)ferrocene, preparation 97239-80-0DP, 1,1'-Bis(disopropylphosphino)ferrocene, **rhodium complex**.
 RL: CAT (Catalyst use); IMF (Industrial manufacture); PREP (Preparation); USES (Uses)
 (supported ferrocene-based catalysts for selective **aldehyde hydrogenation**)

IT 71-41-0P, n-Pentanol, preparation 505-10-2P 619-73-8P, p-Nitrobenzyl alcohol 636-72-6P, Thiophene-2-methanol 873-75-6P, p-Bromobenzyl alcohol 3446-90-0P, p-Methylthiobenzyl alcohol 6214-45-5P, p-Butoxybenzyl alcohol 79757-77-0P, 4-Bromo-Thiophene-2-methanol

RL: IMF (Industrial manufacture); PREP (Preparation)
 (supported ferrocene-based catalysts for selective **aldehyde hydrogenation**)

IT 98-03-3, 2-Formylthiophene 110-62-3, Pentanal
 555-16-8, p-Nitrobenzaldehyde, reactions
 1122-91-4, p-Bromobenzaldehyde 3268-49-3
 3446-89-7, p-Thiomethylbenzaldehyde 5736-88-9, p-Butoxybenzaldehyde 18791-75-8, 4-Bromo-2-Formylthiophene
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (supported ferrocene-based catalysts for selective **aldehyde hydrogenation**)

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

- (1) Burk, M; TETRAHEDRON LETTERS 1994, V35(28), P4963 HCPLUS
- (2) Pugin, B; US 5783715 A 1998 HCPLUS
- (3) Seton Hall University; WO 9828074 A 1998 HCPLUS

IT 255064-36-9

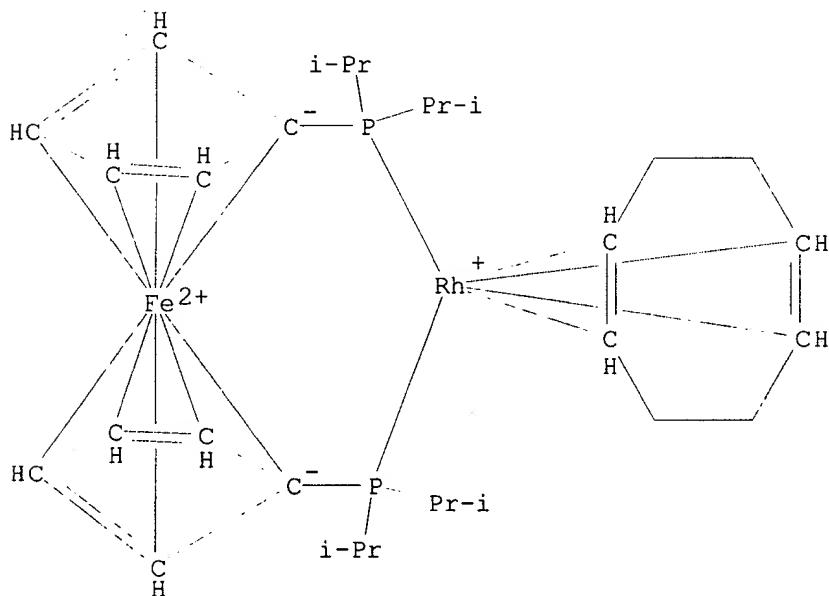
RL: CAT (Catalyst use); USES (Uses)
 (supported ferrocene-based catalysts for selective **aldehyde hydrogenation**)

RN 255064-36-9 HCPLUS

CN Rhodium(1+), [1,1'-bis[bis(1-methylethyl)phosphino-
 κP]ferrocene][(1,2,5,6-η)-1,5-cyclooctadiene]-,
 tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

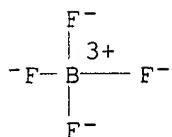
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CRN 157772-65-1
 CMF C30 H48 Fe P2 Rh
 CCI CCS



CM 2

CRN 14874-70-5
 CMF B F4
 CCI CCS

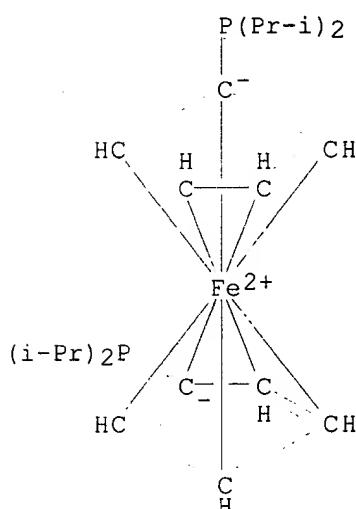


IT 97239-80-0DP, 1,1'-Bis(diisopropylphosphino)ferrocene,
rhodium complex

RL: CAT (Catalyst use); IMF (Industrial manufacture); PREP (Preparation);
USES (Uses)
(supported ferrocene-based catalysts for selective aldehyde

hydrogenation)

RN 97239-80-0 HCPLUS
CN Ferrocene, 1,1'-bis[bis(1-methylethyl)phosphinol- (9CI) (CA INDEX NAME)



IT 98-03-3, 2-Formylthiophene 110-62-3, Pentanal

555-16-8, p-Nitrobenzaldehyde, reactions

1122-91-4, p-Bromobenzaldehyde 3268-49-3

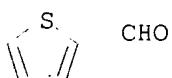
3446-89-7, p-Thiomethylbenzaldehyde

RL: RCT (Reactant); RACT (Reactant or reagent)

REF (Reactant), R₂OR (Reagent or reagent),
(supported ferrocene-based catalysts for selective aldehyde
hydrogenation)

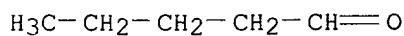
BN 98-03-3 HCAPLUS

RN 55-05-3 HCA-105
CN 2-Thiophenecarboxaldehyde (7CI, 8CI, 9CI) (CA INDEX NAME)



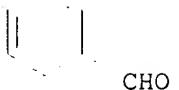
RN 110-62-3 HCAPLUS

CN Pentanal (9CI) (CA INDEX NAME)



RN 555-16-8 HCAPLUS

CN Benzaldehyde, 4-nitro- (9CI) (CA INDEX NAME)

O₂N

RN 1122-91-4 HCAPLUS
 CN Benzaldehyde, 4-bromo- (9CI) (CA INDEX NAME)

CHO



Br

RN 3268-49-3 HCAPLUS
 CN Propanal, 3-(methylthio)- (9CI) (CA INDEX NAME)

MeS—CH₂—CH₂—CHO

RN 3446-89-7 HCAPLUS
 CN Benzaldehyde, 4-(methylthio)- (9CI) (CA INDEX NAME)

CHO



MeS

L104 ANSWER 2 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN
 AN 1999:767776 HCAPLUS
 DN 132:108089
 ED Entered STN: 06 Dec 1999
 TI Phosphines versus phosphinites as ligands in the rhodium
 catalyzed asymmetric **hydrogenation** of imines: a systematic study
 AU Tararov, Vitali I.; Kadyrov, Renat; Riermeier, Thomas H.; Holz, Jens;
 Borner, Armin
 CS Institut fur Organische Katalyseforschung an der Universitat Rostock e.V.,
 Rostock, D-18055, Germany
 SO Tetrahedron: Asymmetry (1999), 10(20), 4009-4015
 CODEN: TASYE3; ISSN: 0957-4166
 PB Elsevier Science Ltd.
 DT Journal
 LA English
 CC 29-13 (Organometallic and Organometalloidal Compounds)
 Section cross-reference(s): 67
 OS CASREACT 132:108089
 AB The asym. **hydrogenation** of N-(1-phenylethylidene)benzylamine
 with a range of Rh(I)-diphosphine and diphosphinite catalysts
 was studied. The reaction is strongly sensitive to the size of the metal
 chelate. Complexes based on five- and six-membered chelates or
 electron-rich alkylphosphines gave poor or moderate conversions. The
 reactivity of diphosphine catalysts could be increased by the addition of
 p-toluenesulfonic acid. Unexpectedly, Rh-complexes based on
 chiral diphosphinites and a diphosphite also rapidly converted the
 substrate to the desired amine. Highest efficiency was observed with a

ST **Rh(I) complex with (R,R)-1,2-cyclohexanol-bisdiphenylphosphinite [(R,R)-bdpch] as chiral ligand. Without any additive complete hydrogenation of the imine was achieved within 5 h. The product was produced in an enantioselectivity of 71%.**

ST phosphine phosphinites ligand comparison **rhodium** catalyzed asym **hydrogenation** imine

IT Phosphines
RL: CAT (Catalyst use); USES (Uses)
(diphosphines; phosphines vs. phosphinites as ligands in the **rhodium** catalyzed asym. **hydrogenation** of imines: a systematic study)

IT Amines, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(phosphines vs. phosphinites as ligands in the **rhodium** catalyzed asym. **hydrogenation** of imines)

IT Imines
RL: RCT (Reactant); RACT (Reactant or reagent)
(phosphines vs. phosphinites as ligands in the **rhodium** catalyzed asym. **hydrogenation** of imines: a systematic study)

IT **Hydrogenation**
Hydrogenation catalysts
(stereoselective; phosphines vs. phosphinites as ligands in the **rhodium** catalyzed asym. **hydrogenation** of imines: a systematic study)

IT 14428-98-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(: (phosphine)- and (phosphinite) **rhodium**-catalyzed asym. **hydrogenation** of)

IT 53450-79-6 60104-68-9 60430-43-5 63569-12-0 66787-44-8
72611-80-4 79255-71-3 82796-32-5 109143-86-4 163161-28-2
171561-30-1 171561-32-3 180420-80-8 185754-11-4 187886-92-6
204762-36-7 214827-80-2 217818-18-3 237058-40-1 255064-34-7
255064-35-8 255064-36-9 255064-38-1 255064-68-7
255719-90-5
RL: CAT (Catalyst use); USES (Uses)
(phosphines vs. phosphinites as ligands in the **rhodium** catalyzed asym. **hydrogenation** of imines)

IT 17480-69-2P 38235-77-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RE.CNT 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

- (1) Achiwa, K; J Am Chem Soc 1976, V98, P8265 HCPLUS
- (2) Bakos, J; J Chem Soc, Chem Commun 1991, P1684 HCPLUS
- (3) Bomer, A; Tetrahedron Lett 1994, V35, P6071
- (4) Borns, S; Eur J Inorg Chem 1998, P1291 HCPLUS
- (5) Borns, S; Tetrahedron: Asymmetry 1999, V10, P1425 HCPLUS
- (6) Broger, E; Tetrahedron: Asymmetry 1998, V9, P4043 HCPLUS
- (7) Burk, M; J Am Chem Soc 1992, V114, P6266 HCPLUS
- (8) Cahill, J; Tetrahedron: Asymmetry 1998, V9, P4307 HCPLUS
- (9) Cullen, W; J Mol Catal 1990, V62, P243 HCPLUS
- (10) Cullen, W; J Mol Catal 1990, V62, P243 HCPLUS
- (11) Holz, J; Tetrahedron: Asymmetry 1995, V6, P1973 HCPLUS
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- (13) Kadyrov, R; Tetrahedron: Asymmetry 1998, V9, P329 HCPLUS
- (14) Kagan, H; J Am Chem Soc 1972, V94, P6429 HCPLUS
- (15) Kobayashi, S; Chem Rev 1999, V99, P1069 HCPLUS
- (16) Krause, H; J Mol Catal A: Chemical 1995, V104, P147 HCPLUS
- (17) Krause, H; New J Chem 1989, V13, P615 HCPLUS
- (18) Kumar, A; Angew Chem 1994, V106, P2272 HCPLUS
- (19) Kumar, A; Angew Chem, Int Ed Engl 1994, V33, P2197
- (20) Lensink, C; Tetrahedron: Asymmetry 1992, V3, P235 HCPLUS
- (21) Morimoto, T; Tetrahedron: Asymmetry 1995, V6, P2661 HCPLUS

(22) Ng Cheon Chan, Y; J Am Chem Soc 1990, V112, P940
 (23) Noyori, R; Asymmetric Catalysis in Organic Synthesis 1994, P82
 (24) Ojima, I; Catalytic Asymmetric Synthesis 1993, P31
 (25) Ringwald, M; J Am Chem Soc 1999, V121, P1524 HCPLUS
 (26) Sablone, R; Tetrahedron Lett 1997, V37, P4937
 (27) Sablone, R; Tetrahedron: Asymmetry 1996, V7, P3059 HCPLUS
 (28) Schnider, P; Chem Eur J 1997, V3, P887 HCPLUS
 (29) Selke, R; J Mol Catal 1986, V37, P213 HCPLUS
 (30) Selke, R; Tetrahedron 1996, V52, P15079 HCPLUS
 (31) Spindler, F; Angew Chem 1990, V102, P561 HCPLUS
 (32) Spindler, F; Angew Chem, Int Ed Engl 1990, V29, P558
 (33) Spindler, F; Transition Metals for Organic Synthesis 1998, V2, P69 HCPLUS
 (34) Tanaka, M; J Chem Soc, Chem Commun 1975, P735 HCPLUS
 (35) Tani, K; Chem Lett 1995, P955 HCPLUS
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 (37) Trinkhaus, S; J Mol Catal A: Chemical 1999, V144, P15 HCPLUS
 (38) Trinkhaus, S; Tetrahedron Lett 1997, V38, P807 HCPLUS
 (39) Vastag, S; J Mol Catal 1984, V22, P283 HCPLUS
 (40) Willoughby, C; J Am Chem Soc 1992, V114, P7562 HCPLUS
 (41) Zhu, G; Tetrahedron: Asymmetry 1998, V9, P2415 HCPLUS

IT 255064-35-8 255064-36-9

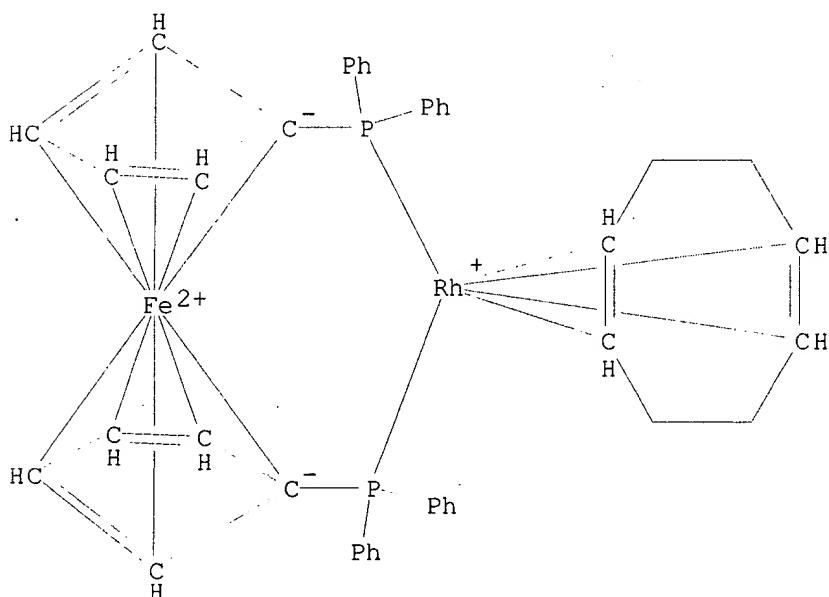
RL: CAT (Catalyst use); USES (Uses)
 (phosphines vs. phosphinites as ligands in the rhodium
 catalyzed asym. **hydrogenation** of imines)

RN 255064-35-8 HCPLUS

CN Rhodium(1+), [1,1'-bis(diphenylphosphino- κ P)ferrocene][(1,2,5,6- η)-1,5-cyclooctadiene]-, tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

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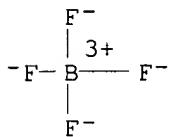
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CRN 14874-70-5
 CMF B F4

CCI CCS



RN 255064-36-9 HCAPLUS

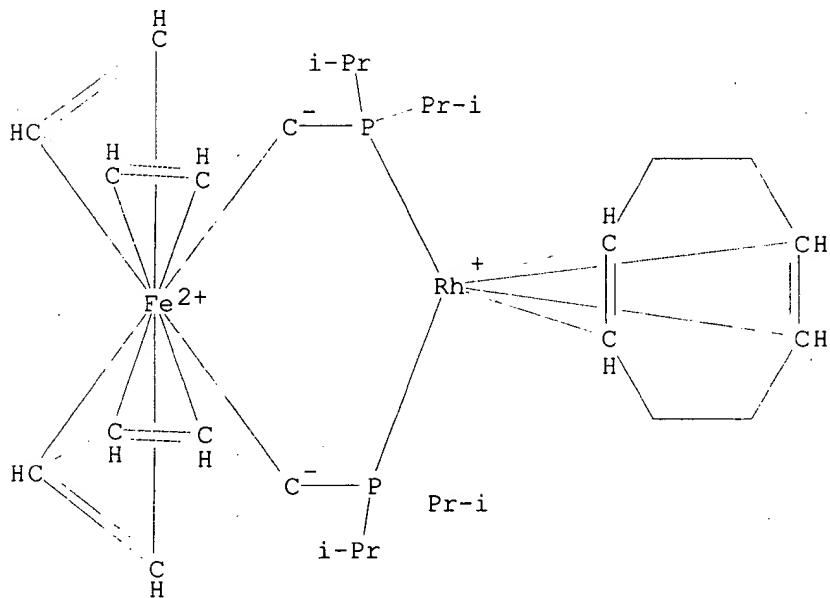
CN Rhodium(1+), [1,1'-bis[bis(1-methylethyl)phosphino-
κP]ferrocene][(1,2,5,6-η)-1,5-cyclooctadiene]-,
tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

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CRN 157772-65-1

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CCI CCS

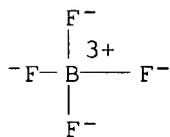


CM 2

CRN 14874-70-5

CMF B F4

CCI CCS



DN 129:303986
 ED Entered STN: 22 Oct 1998
 TI Processes and catalysts for producing **hydroxyaldehydes**
 IN Briggs, John Robert; Packett, Diane Lee; Bryant, David Robert; Phillips, Ailene Gardner; Schreck, David James; Olson, Kurt Damar; Tjaden, Erik Bruce; Guram, Anil Sakharam; Eisenschmid, Thomas Carl; Brigham, Elaine Susan
 PA Union Carbide Chemicals & Technology Corp., USA
 SO U.S., 36 pp.
 CODEN: USXXAM
 DT Patent
 LA English
 IC ICM C07C045-50
 NCL 568454000
 CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5821389	A	19981013	US 1997-843339	19970415 <--
	CN 1222903	A	19990714	CN 1997-195721	19970423 <--
PRAI	US 1997-843339		19970415 <--		

OS MARPAT 129:303986

AB This invention relates in part to processes for producing one or more substituted or unsubstituted **hydroxyaldehydes**, e.g., 6-hydroxyhexanals, which comprise subjecting one or more substituted or unsubstituted alkadienes, e.g., butadiene, to reductive hydroformylation in the presence of a reductive hydroformylation catalyst, e.g., a metal-organophosphorus ligand complex catalyst, and hydroformylation in the presence of a hydroformylation catalyst, e.g., a metal-organophosphorus ligand complex catalyst, to produce one or more substituted or unsubstituted **hydroxyaldehydes**. The substituted and unsubstituted **hydroxyaldehydes** produced by the processes of this invention can undergo further reaction(s) to afford desired derivs. thereof, e.g., epsilon caprolactone. This invention also relates in part to reaction mixts. containing one or more substituted or unsubstituted **hydroxyaldehydes** as principal product(s) of reaction.

ST **hydroxyaldehyde** manuf diene hydroformylation; metal organophosphorus ligand complex catalyst hydroformylation

IT **Aldehydes, preparation**

RL: IMF (Industrial manufacture); PREP (Preparation)
(**hydroxy**; processes and catalysts for producing
hydroxyaldehydes)

IT Hydroformylation

Hydroformylation catalysts
(processes and catalysts for producing **hydroxyaldehydes**)

IT Alkadienes

RL: RCT (Reactant); RACT (Reactant or reagent)
(processes and catalysts for producing **hydroxyaldehydes**)

IT 554-70-1, Triethylphosphine 594-09-2, Trimethylphosphine 603-35-0, Triphenylphosphine, uses 607-01-2, Ethyldiphenylphosphine 998-40-3, Tributylphosphine 1605-53-4, Diethylphenylphosphine 4023-53-4, Tris(2-cyanoethyl)phosphine 4706-17-6 4731-53-7, Trioctylphosphine 6372-40-3, Isopropylidiphenylphosphine 6737-42-4 **12150-46-8**
14874-82-9, **Rhodium** dicarbonyl acetylacetone 17005-57-1
19262-01-2, Cyclohexyldiethylphosphine 32305-98-9 32376-20-8,
t-Butyldiethylphosphine 50420-43-4, n-Butyldiethylphosphine
53111-20-9, Diphenyl(o-methoxyphenyl)phosphine 76189-55-4,
(R)-(+)-2,2'-Bis(diphenylphosphino)-1,1'-binaphthyl **84680-96-6**
108793-33-5 111982-81-1, 2,2'-(Bisdiphenylphosphinomethyl)1,1'-biphenyl
121627-17-6 138776-88-2 138776-89-3 154813-98-6 154814-02-5
169254-16-4 198475-94-4 198478-30-7 198478-33-0

RL: CAT (Catalyst use); USES (Uses)

(processes and catalysts for producing **hydroxyaldehydes**)

IT 34067-76-0P, 6-Hydroxyhexanal
 RL: IMF (Industrial manufacture); PREP (Preparation)
 (processes and catalysts for producing hydroxyaldehydes)
 IT 764-37-4P, trans-3-Penten-1-ol 764-38-5P, cis-3-Penten-1-ol 821-09-0P,
 4-Penten-1-ol 1576-95-0P, cis-2-Penten-1-ol 1576-96-1P,
 trans-2-Penten-1-ol
 RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT
 (Reactant or reagent)
 (processes and catalysts for producing hydroxyaldehydes)
 IT 106-99-0, Butadiene, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (processes and catalysts for producing hydroxyaldehydes)

RE.CNT 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

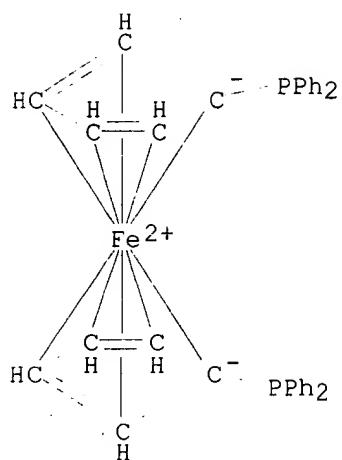
- (1) Anderson, J; Chem Commun 1996, P1543
- (2) Anon; GB 1254222 1971 HCPLUS
- (3) Anon; GB 1357735 1974 HCPLUS
- (4) Anon; EP 0183545 1985 HCPLUS
- (5) Anon; EP 0343819 1989 HCPLUS
- (6) Anon; EP 0420510 1991 HCPLUS
- (7) Anon; EP 0448848 1991 HCPLUS
- (8) Bahrmann; US 5583250 1996 HCPLUS
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- (10) Carlock; US 4185038 1980 HCPLUS
- (11) Carlock; US 4189448 1980 HCPLUS
- (12) Carlock; US 4214109 1980 HCPLUS
- (13) Dennis; US 4482749 1984 HCPLUS
- (14) Dennis; US 4567306 1996 HCPLUS
- (15) Fell; US 5434312 1995 HCPLUS
- (16) Henin; US 4658068 1987 HCPLUS
- (17) Hignett; US 4200591 1980 HCPLUS
- (18) Hignett; US 4200592 1980 HCPLUS
- (19) Hoshiyama; US 4447661 1984 HCPLUS
- (20) Johnson; US 3660493 1972 HCPLUS
- (21) Johnson; US 4409418 1983 HCPLUS
- (22) Kim; US 4198352 1980 HCPLUS
- (23) Knifton; US 4451679 1984 HCPLUS
- (24) Knifton; US 4469895 1984 HCPLUS
- (25) Kummer; US 3947503 1976 HCPLUS
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- (27) Malcolm, J; 1972 HCPLUS
- (28) Mullin; US 5504261 1996 HCPLUS
- (29) Ohyama; US 4376212 1983 HCPLUS
- (30) Oswald; US 4528404 1985 HCPLUS
- (31) Packett; US 5312996 1994 HCPLUS
- (32) Saito; US 4263449 1981 HCPLUS
- (33) Sato; US 5177228 1930 HCPLUS
- (34) Simpson, M; Hamilton/Coordination Chemistry Reviews 1996, V155(163-207), P186
- (35) Slaugh; US 3239566 1966 HCPLUS
- (36) Smith; US 4224255 1980 HCPLUS
- (37) van Vliet; US 4647707 1987 HCPLUS
- (38) Vargas; US 5306848 1994 HCPLUS
- (39) Yates; US 4443638 1984 HCPLUS
- (40) Young; US 4625068 1986 HCPLUS

IT 12150-46-8 84680-96-6

RL: CAT (Catalyst use); USES (Uses)
 (processes and catalysts for producing hydroxyaldehydes)

RN 12150-46-8 HCPLUS

CN Ferrocene, 1,1'-bis(diphenylphosphino)- (9CI) (CA INDEX NAME)



RN 84680-96-6 HCPLUS

CN Rhodium(1+), [(2,3,5,6- η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis(diphenylphosphino- κ P)ferrocene]-, perchlorate (9CI) (CA INDEX NAME)

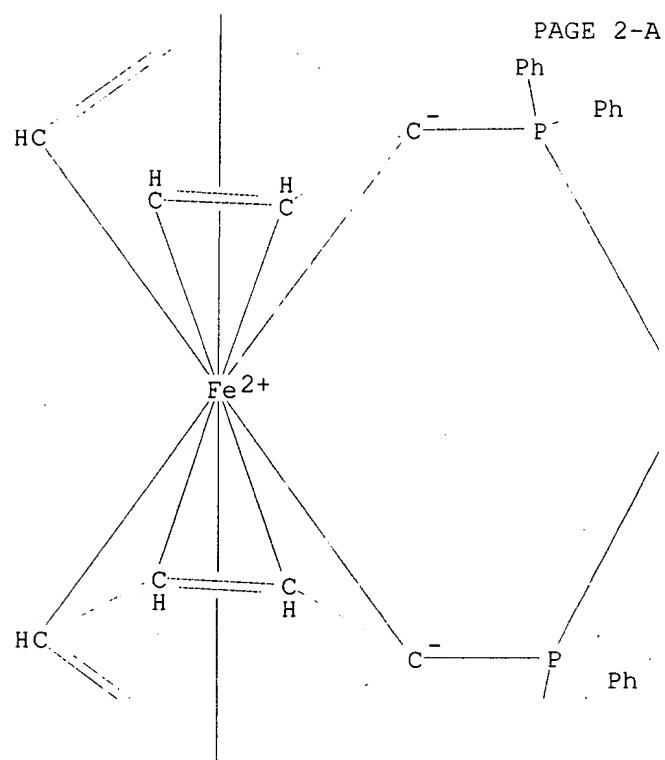
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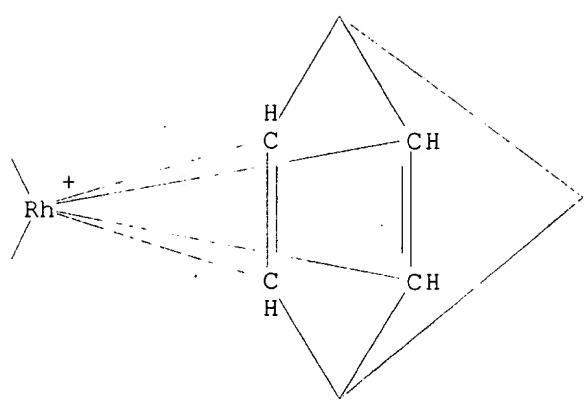
CMF C41 H36 Fe P2 Rh

CCI CCS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *



PAGE 2-B

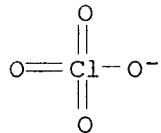


PAGE 3-A

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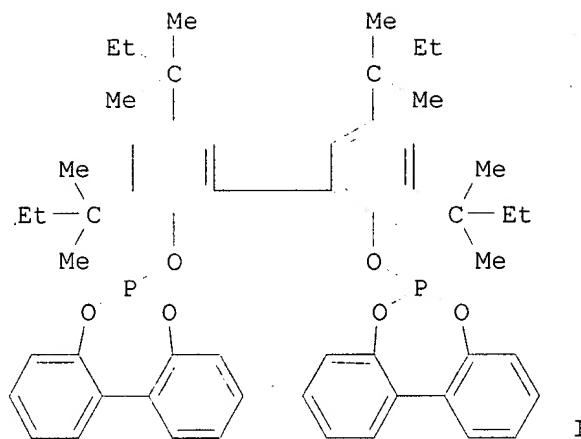
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CMF Cl O4

L104 ANSWER 4 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN
 AN 1997:756953 HCAPLUS
 DN 128:14354
 ED Entered STN: 04 Dec 1997
 TI Selective manufacture of alkenals and alkenols by hydroformylation of alkadienes and catalysts therefor
 IN Packett, Diane Lee; Briggs, John Robert; Bryant, David Robert; Phillips, Ailene Gardner
 PA Union Carbide Chemicals and Plastics Technology Corp., USA
 SO PCT Int. Appl., 109 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 IC C07C045-49; C07C047-21; C07C029-141; C07C033-025
 CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)
 Section cross-reference(s): 67

FAN.CNT 7

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PI	WO 9740002	A1	19971030	WO 1997-US6889	19970423 <--
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	RW: GH, KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	US 5886237	A	19990323	US 1997-843389	19970415 <--
	US 6187970	B1	20010213	US 1997-843390	19970415 <--
	AU 9727422	A1	19971112	AU 1997-27422	19970423 <--
	EP 853609	A1	19980722	EP 1997-921365	19970423 <--
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
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	US 1996-15953P	P	19960424	<--	
	US 1996-16116P	P	19960424	<--	
	US 1996-16287P	P	19960424	<--	
	US 1997-843389	A	19970415	<--	

US 1997-842665 A 19970415 <--
 WO 1997-US6889 W 19970423 <--
 OS MARPAT 128:14354
 GI



AB Substituted or unsubstituted alkadienes, e.g., butadiene, or a mixture thereof are hydroformylated in the presence of a hydroformylation catalyst, e.g., a metal-organophosphorus ligand complex catalyst, and at an alkadiene and/or carbon monoxide partial pressure sufficient to selectively produce ≥ 1 (un)substituted alkenal, e.g., pentenal. The (un)substituted alkenals can undergo further reaction(s) to afford desired derivs., e.g., **hydrogenation** to alkenols, particularly pentenols. The invention also relates to reaction mixts. containing ≥ 1 (un)substituted alkenals or alkenols as principal product(s) of the reactions. Thus, liquid butadiene was charged to a reactor containing a THF solution of **rhodium** dicarbonylacetyletonate (200 ppm Rh) and 6,6'-(3,3',5,5'-tetrakis(1,1-dimethylpropyl)-[1,1'-biphenyl]-1,1'-diyl)bis(dibenzo[d,f][1,3,2]dioxaphosphhepin (I) (12:1 ligand-Rh ratio), heated to 95° and pressurized to 500 psig with 1:1 CO-H₂ to give, after 2 h, 95% butadiene conversion to 3-pentenals 75, 4-pentenals 3, 2-pentenals 5, **valeraldehyde** 7, branched **dialdehyde** 1, and **adipaldehyde** 9%.

ST alkadiene hydroformylation alkenal alkenol manuf; butadiene hydroformylation alkenal alkenol catalyst; **rhodium** phosphine ligand hydroformylation catalyst; pentenal manuf hydroformylation butadiene

IT **Aldehydes, preparation**
 RL: IMF (Industrial manufacture); PREP (Preparation)
 (C5; selective manufacture of **alkenals** and alkenols by hydroformylation of alkadienes and catalysts therefor)

IT **Aldehydes, preparation**
 RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
 (alkenals; selective manufacture of **alkenals** and alkenols by hydroformylation of alkadienes and catalysts therefor)

IT **Alcohols, preparation**
 RL: IMF (Industrial manufacture); PREP (Preparation)
 (alkenols; selective manufacture of alkenals and alkenols by hydroformylation of alkadienes and catalysts therefor)

IT **Dialdehydes**
 RL: BYP (Byproduct); PREP (Preparation)

(formation of; in selective manufacture of alkenals and alkenols by hydroformylation of alkadienes and catalysts therefor)

IT Hydroformylation catalysts
 (selective manufacture of alkenals and alkenols by hydroformylation of alkadienes and catalysts therefor)

IT Alkadienes
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (selective manufacture of alkenals and alkenols by hydroformylation of alkadienes and catalysts therefor)

IT 554-70-1, Triethylphosphine 594-09-2, Trimethylphosphine 603-35-0, Triphenylphosphine, uses 1038-95-5, Tris(p-tolyl)phosphine 4023-53-4, Tris(2-cyanoethyl)phosphine 6372-40-3, Isopropylidiphenylphosphine 6737-42-4 **12150-46-8** 14874-82-9, Rhodium dicarbonyl acetylacetone 32305-98-9 53111-20-9 61806-56-2, Phenylbis(cyanomethyl)phosphine **84680-96-6** 108793-33-5 121627-17-6 138776-88-2 138776-89-3 154813-98-6 198475-94-4
 RL: CAT (Catalyst use); USES (Uses)
 (catalyst; selective manufacture of alkenals and alkenols by hydroformylation of alkadienes and catalysts therefor)

IT **110-62-3P**, **Valeraldehyde** 629-11-8P, 1,6-Hexanediol 1072-21-5P, **Adipaldehyde** 34067-76-0P, 6-Hydroxyhexanal
 RL: BYP (Byproduct); PREP (Preparation)
 (formation of; in selective manufacture of alkenals and alkenols by hydroformylation of alkadienes and catalysts therefor)

IT **96-17-3P**, **2-Methylbutyraldehyde** 25167-67-3P, Butene 100080-07-7P
 RL: BYP (Byproduct); PREP (Preparation)
 (formation of; selective manufacture of alkenals and alkenols by hydroformylation of alkadienes and catalysts therefor)

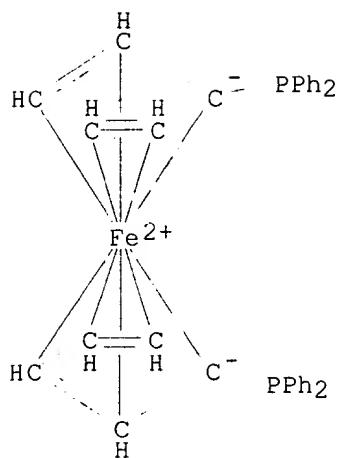
IT 106-99-0, Butadiene, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (hydroformylation of; selective manufacture of alkenals and alkenols by hydroformylation of alkadienes and catalysts therefor)

IT 764-37-4DP, trans-3-Penten-1-ol, derivs. 764-37-4P, trans-3-Penten-1-ol 764-38-5DP, cis-3-Penten-1-ol, derivs. 764-38-5P, cis-3-Penten-1-ol 821-09-0DP, 4-Penten-1-ol, derivs. 821-09-0P, 4-Penten-1-ol 1576-86-9DP, cis-2-Pentenal, derivs. 1576-86-9P, cis-2-Pentenal 1576-87-0DP, trans-2-Pentenal, derivs. 1576-87-0P, trans-2-Pentenal 1576-95-0DP, cis-2-Penten-1-ol, derivs. 1576-95-0P, cis-2-Penten-1-ol 1576-96-1DP, trans-2-Penten-1-ol, derivs. 1576-96-1P, trans-2-Penten-1-ol 2100-17-6DP, 4-Pentenal, derivs. 2100-17-6P, 4-Pentenal 53448-06-9DP, cis-3-Pentenal, derivs. 53448-06-9P 58838-14-5DP, derivs. 58838-14-5P, trans-3-Pentenal
 RL: IMF (Industrial manufacture); PREP (Preparation)
 (selective manufacture of alkenals and alkenols by hydroformylation of alkadienes and catalysts therefor)

IT 106-99-0D, Butadiene, derivs. 630-08-0, Carbon monoxide, reactions 1333-74-0, Hydrogen, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (selective manufacture of alkenals and alkenols by hydroformylation of alkadienes and catalysts therefor)

IT **12150-46-8** **84680-96-6**
 RL: CAT (Catalyst use); USES (Uses)
 (catalyst; selective manufacture of alkenals and alkenols by hydroformylation of alkadienes and catalysts therefor)

RN 12150-46-8 HCAPLUS
 CN Ferrocene, 1,1'-bis(diphenylphosphino)- (9CI) (CA INDEX NAME)



RN 84680-96-6 HCAPLUS

CN Rhodium(1+), [(2,3,5,6- η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis(diphenylphosphino- κ P)ferrocene]-, perchlorate (9CI) (CA INDEX NAME)

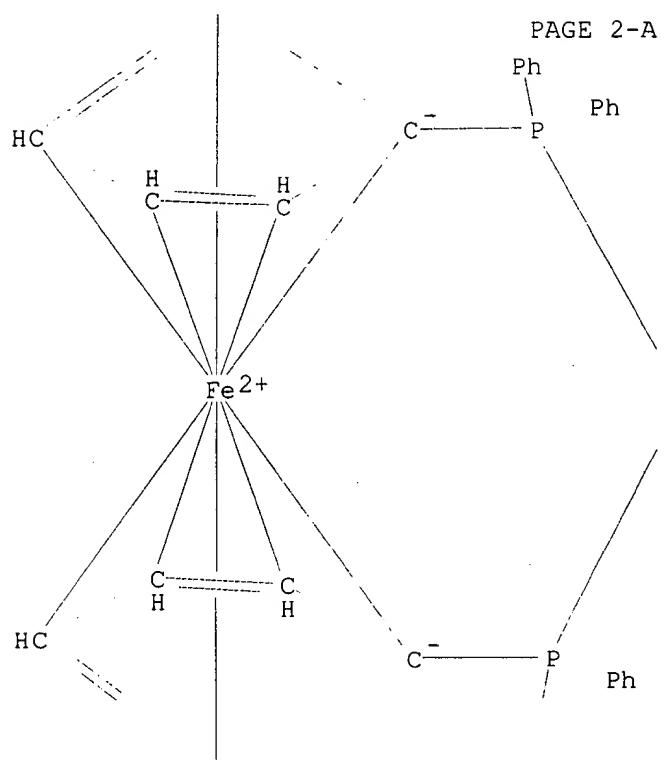
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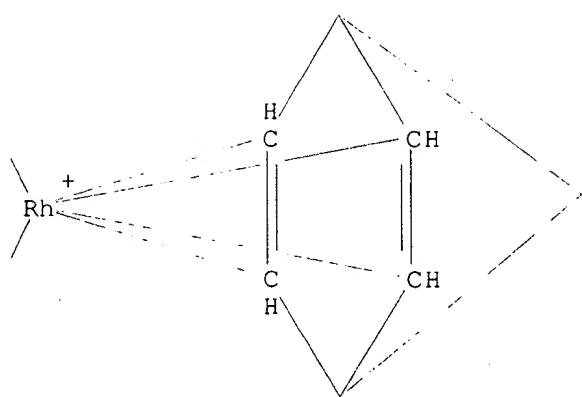
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CCI CCS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *



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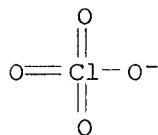


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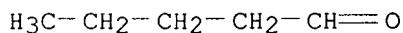
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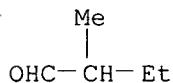
CM 2

CRN 14797-73-0
CMF Cl O4

IT 110-62-3P, **Valeraldehyde**
 RL: BYP (Byproduct); PREP (Preparation)
 (formation of; in selective manufacture of alkenals and alkenols by
 hydroformylation of alkadienes and catalysts therefor)
 RN 110-62-3 HCPLUS
 CN Pentanal (9CI) (CA INDEX NAME)



IT 96-17-3P, **2-Methylbutyraldehyde**
 RL: BYP (Byproduct); PREP (Preparation)
 (formation of; selective manufacture of alkenals and alkenols by
 hydroformylation of alkadienes and catalysts therefor)
 RN 96-17-3 HCPLUS
 CN Butanal, 2-methyl- (9CI) (CA INDEX NAME)



L104 ANSWER 5 OF 20 HCPLUS COPYRIGHT 2004 ACS on STN
 AN 1997:756952 HCPLUS
 DN 128:14353
 ED Entered STN: 04 Dec 1997
 TI Manufacture of **hydroxyaldehydes** by hydroformylation of
 alkadienes or pentenals and catalysts therefor
 IN Briggs, John Robert; Packett, Diane Lee; Bryant, David Robert; Phillips,
 Ailene Gardner; Schreck, David James; Olson, Kurt Damar; Tjaden, Erick
 Bruce; Guram, Anil Sakharam; Eisenschmid, Thomas Carl; Braghams, Elaine
 Susan
 PA Union Carbide Chemicals and Plastics Technology Corp., USA
 SO PCT Int. Appl., 113 pp.
 CODEN: PIXXD2

DT Patent

LA English

IC C07C045-49; C07C043-68; C07C029-16; C07C045-50; C07C047-19

CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)

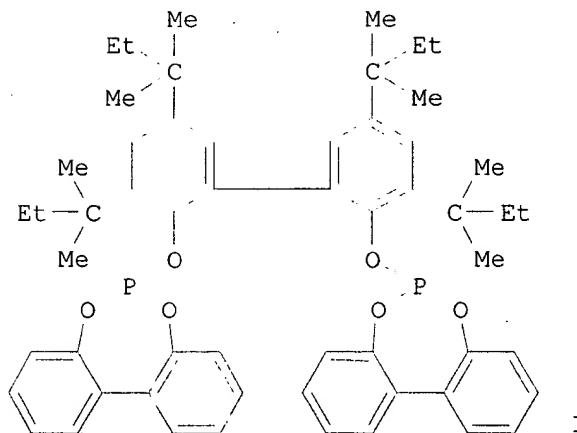
Section cross-reference(s): 35, 67

FAN.CNT 6

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PI	WO 9740001	A1	19971030	WO 1997-US6881	19970423 <--
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	RW: GH, KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
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	US 1996-16259P	P	19960424		<--
	US 1996-16263P	P	19960424		<--
	US 1996-16378P	P	19960424		<--
	US 1997-843340	A	19970415		<--
OS	WO 1997-US6881	W	19970423		<--

OS MARPAT 128:14353

GI



AB Substituted or unsubstituted **hydroxyaldehydes**, e.g., 6-hydroxyhexanals, are prepared by reductive hydroformylation of ≥ 1 (un)substituted alkadienes, e.g., butadiene, or pentenals in the presence of a reductive hydroformylation catalyst; e.g., a metal-organophosphorus

ligand complex catalyst, and hydroformylation of the unsatd. **alcs**. in the presence of a hydroformylation catalyst, e.g., a metal-organophosphorus ligand complex catalyst. The (un)substituted **hydroxylaldehydes** can undergo further reaction(s) to afford desired derivs., e.g., ϵ -caprolactone (no data). Thus, liquid butadiene was charged to a reactor containing a THF solution of **rhodium** dicarbonyl acetylacetone (200 ppm Rh) and 6,6'-[[3,3'5,5'-tetrakis(1,1-dimethylpropyl)[1,1'-biphenyl]-2,2'-diyl]bis(oxy)]bis-dibenzo[d,f][1,3,2]dioxaphosphhepin (I) (12:1 ligand-Rh ratio), heated to 95° and pressurized to 500 psig with 1:1 CO-H₂, giving, after 2 h, 95% butadiene conversion to 3-pentenals 75, 4-pentenal 3, 2-pentenals 5, **valeraldehyde** 7, branched **dialdehyde** 1, and **adipaldehyde** 9%.

ST **hydroxylaldehyde** manuf hydroformylation alkadiene pentenal; **alc**; metal organophosphorus ligand hydroformylation catalyst; butadiene reductive hydroformylation catalyst **hydroxylaldehyde** manuf; **rhodium** dicarbonyl acetylacetone hydroformylation catalyst; phosphine ligand hydroformylation catalyst

IT **Aldehydes, preparation**
RL: IMF (Industrial manufacture); PREP (Preparation)
(C5, preparation of; in manufacture of **hydroxylaldehydes** by hydroformylation of alkadienes, pentenals or unsatd. **alcs.** and catalysts therefor)

IT **Dialdehydes**
RL: BYP (Byproduct); PREP (Preparation)
(branched, formation of; in manufacture of **hydroxylaldehydes** by hydroformylation of alkadienes, pentenals or unsatd. **alcs.** and catalysts therefor)

IT **Aldehydes, preparation**
RL: IMF (Industrial manufacture); PREP (Preparation)
(**hydroxy**; manufacture of **hydroxylaldehydes** by hydroformylation of alkadienes, pentenals or unsatd. **alcs.** and catalysts therefor)

IT **Hydroformylation catalysts**
(manufacture of **hydroxylaldehydes** by hydroformylation of alkadienes, pentenals or unsatd. **alcs.** and catalysts therefor)

IT **Alkadienes**
RL: RCT (Reactant); RACT (Reactant or reagent)
(manufacture of **hydroxylaldehydes** by hydroformylation of alkadienes, pentenals or unsatd. **alcs.** and catalysts therefor)

IT **Alcohols, reactions**
RL: RCT (Reactant); RACT (Reactant or reagent)
(unsatd.; manufacture of **hydroxylaldehydes** by hydroformylation of alkadienes, pentenals or unsatd. **alcs.** and catalysts therefor)

IT **96-17-3P, 2-Methylbutyraldehyde 110-62-3P,**
Valeraldehyde 764-39-6P, 2-Pentenal 1072-21-5P,
Adipaldehyde 2100-17-6P, 4-Pentenal 5604-55-7P, 3-Pentenal 25167-67-3P, Butene 100080-07-7P
RL: BYP (Byproduct); PREP (Preparation)
(byproduct; manufacture of **hydroxylaldehydes** by hydroformylation of alkadienes or pentenals and catalysts therefor)

IT 71-41-0DP, Pentan-1-ol, derivs. 110-62-3DP,
Valeraldehyde, derivs. 111-30-8DP, 1,5-Pantanediol, derivs. 638-37-9DP, 1,4-Butanediol, derivs. 1072-21-5DP, 1,6-Hexanediol, derivs.
RL: BYP (Byproduct); PREP (Preparation)
(byproduct; manufacture of **hydroxylaldehydes** by hydroformylation of alkadienes, pentenals or unsatd. **alcs.** and catalysts therefor)

IT 594-09-2, Trimethylphosphine 603-35-0, Triphenylphosphine, uses

607-01-2, Ethyldiphenylphosphine 672-66-2 1038-95-5,
 Tris(p-tolyl)phosphine 1605-53-4, Diethylphenylphosphine 2234-97-1,
 Tripropylphosphine 4023-53-4, Tris(2-cyanoethyl)phosphine 4731-53-7,
 Trioctylphosphine 6372-40-3, Isopropyldiphenylphosphine 6737-42-4
12150-46-8 14874-82-9, **Rhodium** dicarbonyl
 acetylacetone 19262-01-2 32305-98-9 32376-20-8,
 tert-Butyldiethylphosphine 50420-43-4 53111-20-9 **84680-96-6**
 108793-33-5 121627-17-6 138776-88-2 138776-89-3 154813-98-6
 198475-94-4
 RL: CAT (Catalyst use); USES (Uses)
 (catalyst; manufacture of **hydroxyaldehydes** by hydroformylation of
 alkadienes or pentenals and catalysts therefor)
 IT 19584-30-6, **Tetrarhodium** dodecacarbonyl 76189-55-4
 111982-81-1, 2,2'-(Bisdiphenylphosphinomethyl)-1,1'-biphenyl 154814-02-5
 169254-16-4 198478-30-7 198478-33-0 198478-35-2
 RL: CAT (Catalyst use); USES (Uses)
 (catalyst; manufacture of **hydroxyaldehydes** by hydroformylation of
 unsatd. **alcs.** and catalysts therefor)
 IT 764-37-4P, trans-3-Penten-1-ol 60544-74-3P, 2-Pentenol
 RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT
 (Reactant or reagent)
 (formation and reaction of; manufacture of **hydroxyaldehydes** by
 hydroformylation of unsatd. **alcs.** and catalysts therefor)
 IT 71-41-0P, 1-Pentanol, preparation
 RL: BYP (Byproduct); PREP (Preparation)
 (formation in hydroformylation of cis-3-pentenol; manufacture of
hydroxyaldehydes by hydroformylation of unsatd. **alcs.**
 and catalysts therefor)
 IT 106-99-0D, Butadiene, derivs.
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (manufacture of **hydroxyaldehydes** by hydroformylation of alkadienes
 and catalysts therefor)
 IT 106-99-0, Butadiene, reactions 630-08-0, Carbon monoxide, reactions
 1333-74-0, Hydrogen, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (manufacture of **hydroxyaldehydes** by hydroformylation of alkadienes
 or pentenals and catalysts therefor)
 IT 4221-03-8DP, 5-Hydroxypentanal, derivs. 4221-03-8P, 5-Hydroxypentanal
 25714-71-0DP, 4-Hydroxybutanal, derivs. 25714-71-0P, 4-Hydroxybutanal
 34067-76-0DP, 6-Hydroxyhexanal, derivs. 34067-76-0P, 6-Hydroxyhexanal
 RL: IMF (Industrial manufacture); PREP (Preparation)
 (manufacture of **hydroxyaldehydes** by hydroformylation of
 alkadienes, pentenals or unsatd. **alcs.** and catalysts
 therefor)
 IT 31424-04-1D, Pentenal, derivs.
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (manufacture of **hydroxyaldehydes** by hydroformylation of
 alkadienes, pentenals or unsatd. **alcs.** and catalysts
 therefor)
 IT 764-38-5, cis-3-Pentenol
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (manufacture of **hydroxyaldehydes** by hydroformylation of unsatd.
alcs. and catalysts therefor)
 IT 156619-80-6P, Penten-1-ol
 RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and reaction of; manufacture of **hydroxyaldehydes** by
 hydroformylation of alkadienes, pentenals or unsatd. **alcs.**
 and catalysts therefor)
 IT 156619-80-6D, Penten-1-ol, derivs.
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation and reaction of; manufacture of **hydroxyaldehydes** by
 hydroformylation of alkadienes, pentenals or unsatd. **alcs.**

and catalysts therefor)

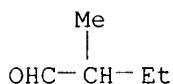
IT 821-09-0P, 4-Pentenol 1576-95-0P, cis-2-Penten-1-ol 1576-96-1P,
trans-2-Penten-1-ol
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and reaction of; manufacture of **hydroxyaldehydes** by
hydroformylation of unsatd. **alcs.** and catalysts therefor)

IT 695-06-7P 18545-19-2P
RL: IMF (Industrial manufacture); PREP (Preparation)
(preparation of; manufacture of **hydroxyaldehydes** by hydroformylation of
unsatd. **alcs.** and catalysts therefor)

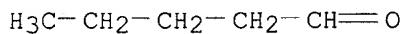
IT 96-17-3P, 2-Methylbutyraldehyde 110-62-3P,
Valeraldehyde
RL: BYP (Byproduct); PREP (Preparation)
(byproduct; manufacture of **hydroxyaldehydes** by hydroformylation of
alkadienes or pentenals and catalysts therefor)

RN 96-17-3 HCAPLUS

CN Butanal, 2-methyl- (9CI) (CA INDEX NAME)

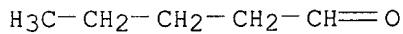


RN 110-62-3 HCAPLUS
CN Pentanal (9CI) (CA INDEX NAME)

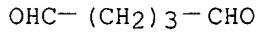


IT 110-62-3DP, **Valeraldehyde**, derivs. 111-30-8DP,
1,5-Pentanodial, derivs.
RL: BYP (Byproduct); PREP (Preparation)
(byproduct; manufacture of **hydroxyaldehydes** by hydroformylation of
alkadienes, pentenals or unsatd. **alcs.** and catalysts
therefor)

RN 110-62-3 HCAPLUS
CN Pentanal (9CI) (CA INDEX NAME)

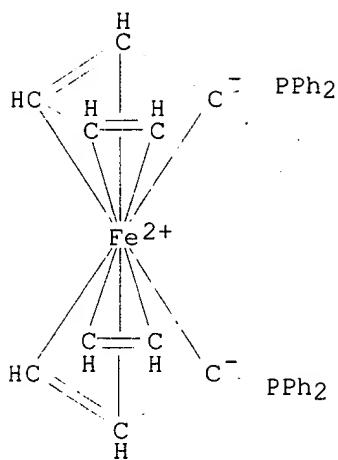


RN 111-30-8 HCAPLUS
CN Pentanodial (9CI) (CA INDEX NAME)



IT 12150-46-8 84680-96-6
RL: CAT (Catalyst use); USES (Uses)
(catalyst; manufacture of **hydroxyaldehydes** by hydroformylation of
alkadienes or pentenals and catalysts therefor)

RN 12150-46-8 HCAPLUS
CN Ferrocene, 1,1'-bis(diphenylphosphino)- (9CI) (CA INDEX NAME)



RN 84680-96-6 HCAPLUS

CN Rhodium(1+), [(2,3,5,6- η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis(diphenylphosphino- κ P)ferrocene]-, perchlorate (9CI) (CA INDEX NAME)

CM 1

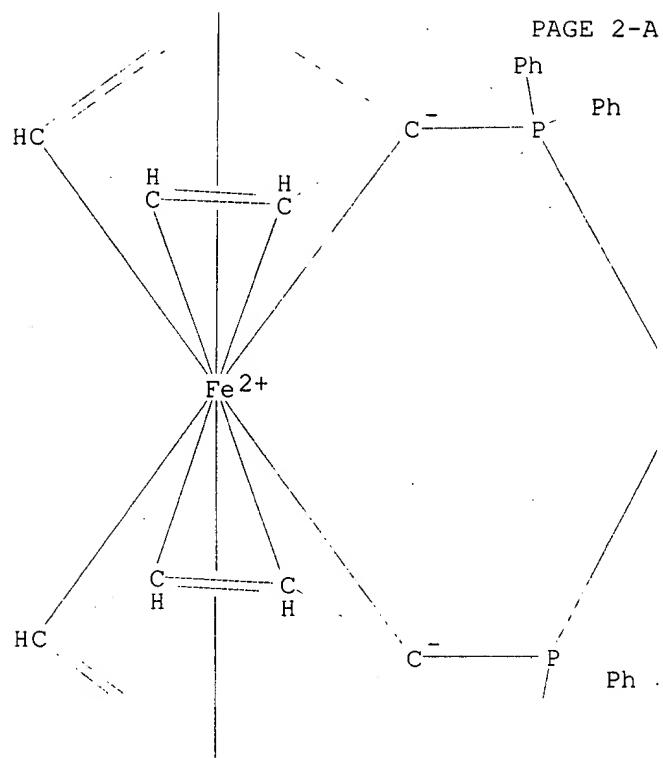
CRN 79790-97-9

CMF C41 H36 Fe P2 Rh

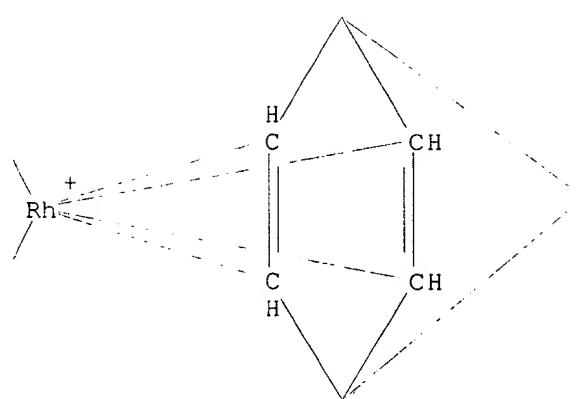
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* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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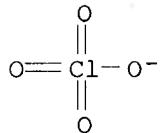


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Ph

C
H

CM 2

CRN 14797-73-0
CMF Cl O4

L104 ANSWER 6 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN
 AN 1997:740058 HCAPLUS
 DN 128:13065
 ED Entered STN: 24 Nov 1997
 TI Preparation of alkenols by reductive hydroformylation of alkadienes.
 IN Packett, Diane Lee; Briggs, John Robert; Bryant, David Robert; Phillips, Ailene Gardner; Schreck, David James; Guram, Anil Sakharam; Olson, Kurt Dawar; Eisenschmid, Thomas Carl; Tjaden, Erik Bruce
 PA Union Carbide Chemicals and Plastics Technology Corp., USA
 SO PCT Int. Appl., 103 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 IC C07C029-16; C07C031-20
 CC 23-7 (Aliphatic Compounds)
 FAN.CNT 7

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9739996	A1	19971030	WO 1997-US6852	19970423 <--
	W: AL, AM, AU, BB, BG, BR, CA, CN, CZ, EE, GE, HU, IS, JP, KG, KP, KR, LK, LR, LT, LV, MD, MG, MN, MX, NO, NZ, PL, RO, SG, SI, SK, TR, TT, UA, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	US 6187970	B1	20010213	US 1997-843390	19970415 <--
	US 2002007096	A1	20020117	US 1997-842666	19970415 <--
	AU 9728093	A1	19971112	AU 1997-28093	19970423 <--
	US 6369283	B1	20020409	US 2000-704411	20001102 <--
PRAI	US 1996-15947P	P	19960424	<--	
	US 1996-16287P	P	19960424	<--	
	US 1997-842666	A	19970415	<--	
	US 1997-843381	A3	19970415	<--	
	WO 1997-US6852	W	19970423	<--	
OS	CASREACT 128:13065; MARPAT 128:13065				
AB	Catalytic reductive hydroformylation of ≥ 1 alkadiene selectively produces ≥ 1 (substituted) alkenol. Thus, a solution of				

rhodium dicarbonyl acetylacetone and trioctylphosphine in octanol was pressurized with butadiene and 600 psi CO/200 psi H₂ and heated at 80° to give 98% butadiene conversion and 88% selectivity for 3- and 4-pentenols.

ST butadiene reductive hydroformylation; alkenol prepn; pentenol prepn; alkadiene reductive hydroformylation

IT **Alcohols, preparation**
 RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
 (alkenols; preparation of alkenols by reductive hydroformylation of alkadienes)

IT **Hydroformylation catalysts**
 (dicarbonylacetylacetone⁺rhodium(I) with phosphine ligands for reductive hydroformylation; preparation of alkenols by reductive hydroformylation of alkadienes)

IT **Alkadienes**
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation of alkenols by reductive hydroformylation of alkadienes)

IT **Hydroformylation**
 (reductive hydroformylation; preparation of alkenols by reductive hydroformylation of alkadienes)

IT 71-41-0P, 1-Pentanol, preparation 110-62-3P,
Valeraldehyde 1576-86-9DP, cis-2-Pentenal, substituted 1576-86-9P, cis-2-Pentenal 1576-87-0DP, trans-2-Pentenal, substituted 1576-87-0P, trans-2-Pentenal 2100-17-6DP, 4-Pentenal, substituted 2100-17-6P, 4-Pentenal 53448-06-9DP, cis-3-Pentenal, substituted 53448-06-9P, cis-3-Pentenal 58838-14-5DP, substituted 58838-14-5P
 RL: BYP (Byproduct); PREP (Preparation)
 (preparation of alkenols by reductive hydroformylation of alkadienes)

IT 554-70-1, Triethylphosphine 594-09-2, Trimethylphosphine 603-35-0, Triphenylphosphine, uses 607-01-2, Ethyldiphenylphosphine 1038-95-5, Tris(p-tolyl)phosphine 1605-53-4, Diethylphenylphosphine 4023-53-4, Tris(2-cyanoethyl)phosphine 4706-17-6, Tris(3-hydroxypropyl)phosphine 4731-53-7, Trioctylphosphine 6372-40-3, Isopropyldiphenylphosphine 6737-42-4 10210-68-1, Dicobalt octacarbonyl 12150-46-8
 14874-82-9, **Rhodium** dicarbonylacetylacetone 17005-57-1
 19262-01-2 32305-98-9D, **rhodium** complex 32376-20-8, tert-Butyldiethylphosphine 50420-43-4 53111-20-9 60576-58-1
 61806-56-2 84680-96-6 108793-33-5 121627-17-6 138776-88-2
 138776-89-3 154813-98-6 198475-94-4
 RL: CAT (Catalyst use); USES (Uses)
 (preparation of alkenols by reductive hydroformylation of alkadienes)

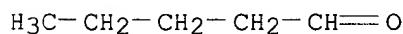
IT 764-37-4DP, trans-3-Penten-1-ol, substituted 764-37-4P, trans-3-Penten-1-ol 764-38-5DP, cis-3-Penten-1-ol, substituted 764-38-5P, cis-3-Penten-1-ol 821-09-0DP, 4-Penten-1-ol, substituted 821-09-0P, 4-Pentenol 1576-95-0DP, cis-2-Penten-1-ol, substituted 1576-95-0P, cis-2-Penten-1-ol 1576-96-1DP, trans-2-Penten-1-ol, substituted 1576-96-1P, trans-2-Penten-1-ol 77035-93-9P, 3-Pentenol
 RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
 (preparation of alkenols by reductive hydroformylation of alkadienes)

IT 106-99-0, Butadiene, reactions 106-99-0D, Butadiene, substituted
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation of alkenols by reductive hydroformylation of alkadienes)

IT 110-62-3P, **Valeraldehyde**
 RL: BYP (Byproduct); PREP (Preparation)
 (preparation of alkenols by reductive hydroformylation of alkadienes)

RN 110-62-3 HCPLUS

CN Pentanal (9CI) (CA INDEX NAME)



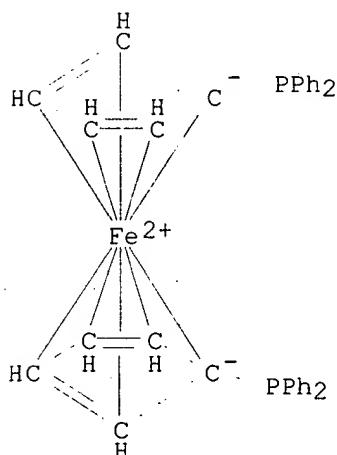
IT 12150-46-8 84680-96-6

RL: CAT (Catalyst use); USES (Uses)

(preparation of alkenols by reductive hydroformylation of alkadienes)

RN 12150-46-8 HCPLUS

CN Ferrocene, 1,1'-bis(diphenylphosphino)- (9CI) (CA INDEX NAME)



RN 84680-96-6 HCPLUS

CN Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis(diphenylphosphino-κP)ferrocene]-, perchlorate (9CI) (CA INDEX NAME)

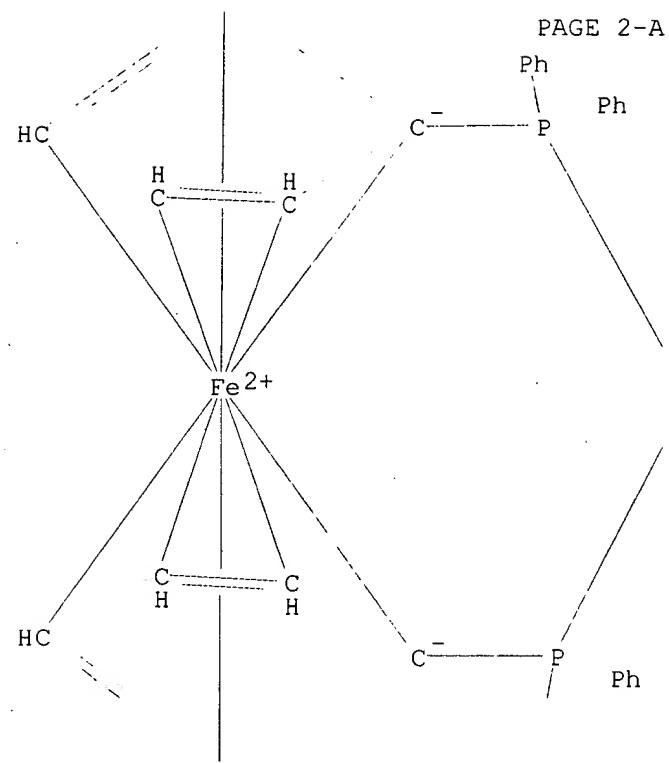
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CRN 79790-97-9

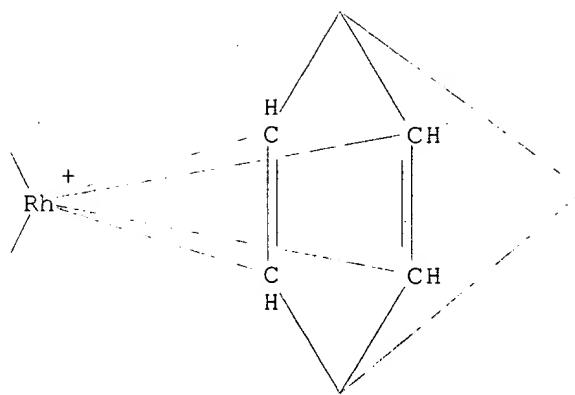
CMF C41 H36 Fe P2 Rh

CCI CCS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *



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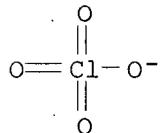
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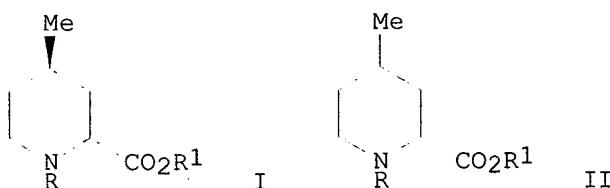
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CRN 14797-73-0
CMF Cl O4

L104 ANSWER 7 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN
 AN 1997:733038 HCAPLUS
 DN 127:358790
 ED Entered STN: 21 Nov 1997
 TI New method for preparing 2,4-trans-disubstituted piperidine derivatives
 IN Grell, Wolfgang
 PA Grell, Wolfgang, Germany
 SO Ger. Offen., 30 pp.
 CODEN: GWXXBX
 DT Patent
 LA German
 IC ICM C07D211-60
 ICS C07B053-00
 ICA C07D211-78; B01J031-24; B01J031-22
 ICI C07M007-00; B01J023-46, B01J105-12
 CC 27-16 (Heterocyclic Compounds (One Hetero Atom))

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 19616049	A1	19971030	DE 1996-19616049	19960423 <--
PRAI	DE 1996-19616049		19960423 <--		
OS	CASREACT 127:358790; MARPAT 127:358790				
GI					



AB Piperidines I [R = H, protective group; R¹ = H, alkyl, protective group] were prepared by hydrogenation of tetrahydropyridines II [R =

protective group; R1 = alkyl, protective group] in presence of a Rh or Ru catalyst. Thus, PhCHMeN:CHCO₂Et was cyclized with isoprene to give II [R = CHMePh, R1 = Et] which was **hydrogenated** over **rhodium(I)** [1,4-bis(diphenylphosphino)butane]-1c,5c-cyclooctadiene tetrafluoroborate followed by hydrogenolysis over Pd-C to give (2R,4R)-I [R = H, R1 = Et] with 93.6% de.

ST tetrahydropyridine stereoselective **hydrogenation** catalysts; piperidine disubstituted stereoselective prepn

IT **Hydrogenation catalysts**

(stereoselective; preparation of 2,4-trans-disubstituted piperidine derivs. by stereoselective **hydrogenation**)

IT 7440-05-3, Palladium, uses 7440-16-6, Rhodium, uses 12122-73-5 12257-42-0 12279-09-3 14694-95-2, Tris(triphenylphosphine)rhodium chloride 15529-49-4 32761-50-5 32799-32-9 32965-49-4 35138-22-8 60576-58-1 62827-87-6 65012-74-0 79255-71-3 **84680-96-6** 126420-28-8 128363-26-8 130004-33-0 145926-28-9 198641-64-4

RL: CAT (Catalyst use); USES (Uses)

(preparation of 2,4-trans-disubstituted piperidine derivs. by stereoselective **hydrogenation**)

IT 78-79-5, reactions 100-46-9, Benzylamine, reactions **924-44-7**, Ethyl glyoxylate 2627-86-3, (S)-1-Phenylethylamine 35823-28-0

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of 2,4-trans-disubstituted piperidine derivs. by stereoselective **hydrogenation**)

IT 37662-06-9P 127897-25-0P 139334-63-7P 145774-82-9P 198641-56-4P 198641-60-0P 198641-62-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of 2,4-trans-disubstituted piperidine derivs. by stereoselective **hydrogenation**)

IT 74892-82-3P 78306-52-2P 79199-61-4P 139359-60-7P 145774-81-8P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of 2,4-trans-disubstituted piperidine derivs. by stereoselective **hydrogenation**)

IT **84680-96-6**

RL: CAT (Catalyst use); USES (Uses)

(preparation of 2,4-trans-disubstituted piperidine derivs. by stereoselective **hydrogenation**)

RN 84680-96-6 HCAPLUS

CN Rhodium(1+), [(2,3,5,6- η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis(diphenylphosphino- κ P)ferrocene]-, perchlorate (9CI) (CA INDEX NAME)

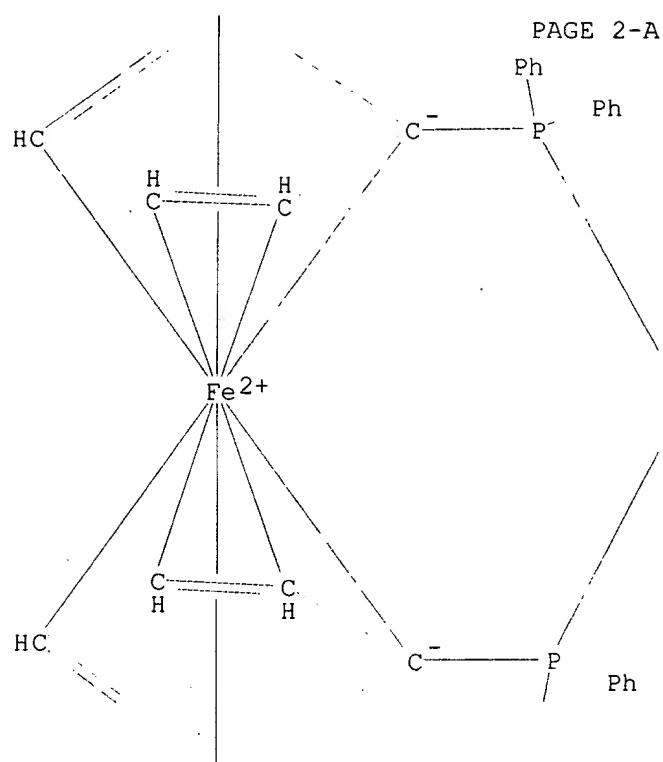
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CRN 79790-97-9

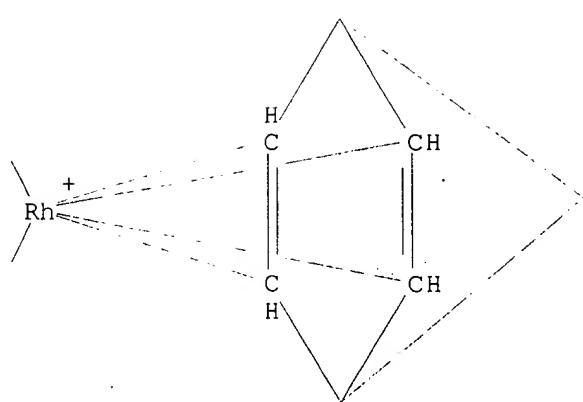
CMF C41 H36 Fe P2 Rh

CCI CCS

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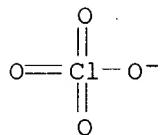
PAGE 3-A

Ph

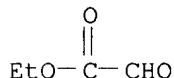
C

H

CM 2

CRN 14797-73-0
CMF Cl 04

IT 924-44-7, Ethyl glyoxylate
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation of 2,4-trans-disubstituted piperidine derivs. by
 stereoselective hydrogenation)
 RN 924-44-7 HCAPLUS
 CN Acetic acid, oxo-, ethyl ester (9CI) (CA INDEX NAME)



L104 ANSWER 8 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN
 AN 1997:57590 HCAPLUS
 DN 126:144405
 ED Entered STN: 27 Jan 1997
 TI Group 9 metal 1,1'-bis(phosphino)ferrocene complexes: synthesis,
 structures, solution conformation and unusual reactivity
 AU Avent, Anthony G.; Bedford, Robin B.; Chaloner, Penny A.; Dewa, Shaliza
 Z.; Hitchcock, Peter B.
 CS School Chem. and Molecular Sciences, Univ. Sussex, Brighton, BN1 9QJ, UK
 SO Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry
 (1996), (24), 4633-4638
 CODEN: JCDTBI; ISSN: 0300-9246
 PB Royal Society of Chemistry
 DT Journal
 LA English
 CC 29-13 (Organometallic and Organometalloidal Compounds)
 Section cross-reference(s): 75
 AB The crystal structure of $[\text{Ir}(\text{cod})(\text{L-L})]^{+}$ (3) [$\text{cod} = \text{cycloocta-1,5-diene}$,
 $\text{L-L} = 1\text{-(diisopropylphosphino)-1'-(diphenylphosphino)ferrocene}$] can be
 related to those of the analogous complexes with $\text{L-L} =$
 $1,1'\text{-bis(diphenylphosphino)ferrocene (dppf) 1 and }1,1'\text{-}$
 $\text{bis(diisopropylphosphino)ferrocene (disoppf), 2, all the complexes being}$
 $\text{readily synthesized from }[\text{Ir}(\text{cod})(\text{py})_2]^{+} (\text{py} = \text{pyridine}). \text{ An optimum}$
 $\text{diphosphine bite angle of .apprx.99}^{\circ} \text{ is maintained in all three}$

complexes by varying the twist of the ferrocene, which decreases with increasing steric profile of the phosphine, and by distortion of the geometry at the Ir atom away from square planar towards tetrahedral. The twist about the ferrocene moiety induces chirality at the Ir atom in all three complexes and the interchange of stereoisomers can be followed by variable-temperature ^1H NMR spectroscopy. Application of the Eyring equation gave approx. values of $\Delta G_{\text{dbldag.}}$ for this process of 36.1 ± 0.2 , 39.3 ± 0.2 and $34.3 \pm 0.2 \text{ kJ mol}^{-1}$ for 1-3 resp. The ligand disoppf also induces considerable distortion away from square-planar geometry in [Rh(nbd)(disoppf)][BF₄] (4) {nbd = norbornadiene (bicyclo[2.2.1]hepta-2,5-diene)}, as found in a crystal structure determination,

which may account for the unusual lability of the chelating diphosphine. This is demonstrated by its reactions with Ph₂P(CH₂)_nPPh₂ (n = 1 or 2) both of which give [Rh(L-L)₂]⁺. More surprisingly, considering its lability in [Rh(nbd)(dppf)]⁺, dppf also readily displaced disoppf from 4, to give [Rh(nbd)(dppf)][BF₄] (5). The nbd ligand in this complex is not displaced by reaction with an excess of dppf.

ST crystal structure iridium **rhodium** bisphosphinoferrocene diene; mol structure iridium **rhodium** bisphosphinoferrocene diene; kinetics conformational inversion iridium bisphosphinoferrocene diene; bisphosphinoferrocene iridium **rhodium** complex prepn structure; ferrocene bisphosphino iridium **rhodium** complex prepn; coordinative substitution **rhodium** bisphosphinoferrocene diene complex

IT Crystal structure
Molecular structure
(of iridium and **rhodium** diene bisphosphinoferrocene complexes)

IT Conformational transition
(of iridium bisphosphinoferrocene diene complexes)

IT Substitution reaction, coordinative
(of **rhodium** diene bisphosphinoferrocene complex)

IT 56678-60-5, (1,5-Cyclooctadiene)bis(pyridine)iridium(1+)
hexafluorophosphate
RL: RCT (Reactant); RACT (Reactant or reagent)

(coordinative substitution reactions with bisphosphinoferrocenes)

IT 97239-80-0, 1,1'-Bis(diisopropylphosphino)ferrocene
RL: RCT (Reactant); RACT (Reactant or reagent)
(coordinative substitution reactions with iridium and **rhodium** diene complexes)

IT 36620-11-8, Bis(norbornadiene)**rhodium**(1+) tetrafluoroborate
RL: RCT (Reactant); RACT (Reactant or reagent)

(coordinative substitution with bis(diisopropylphosphino)ferrocene)

IT 97239-85-5, 1-Diisopropylphosphino-1'-diphenylphosphinoferrocene
RL: RCT (Reactant); RACT (Reactant or reagent)

(coordinative substitution with iridium COD pyridine complex)

IT 1663-45-2, 1,2-Bis(diphenylphosphino)ethane 2071-20-7,
Bis(diphenylphosphino)methane 12150-46-8, 1,1'-
Bis(diphenylphosphino)ferrocene

RL: RCT (Reactant); RACT (Reactant or reagent)

(coordinative substitution with **rhodium**

bis(diisopropylphosphino)ferrocene diene complex)

IT 53450-77-4P, Bis(bis(diphenylphosphino)methane)**rhodium**(1+)
53450-79-6P, Bis(1,2-bis(diphenylphosphino)ethane)**rhodium**(1+)
tetrafluoroborate 79790-98-0P, (1,1'-
Bis(diphenylphosphino)ferrocene) (norbornadiene)**rhodium**(1+)
tetrafluoroborate

RL: SPN (Synthetic preparation); PREP (Preparation)

(formation by coordinative substitution with

bis(diisopropylphosphino)ferrocene analog)

IT 151705-16-7, (1,1'-Bis(diphenylphosphino)ferrocene) (1,5-

cyclooctadiene) iridium(1+) hexafluorophosphate

RL: PEP (Physical, engineering or chemical process); PRP (Properties);
PROC (Process)

(kinetics of conformational inversion and comparison to other
bisphosphinoferrocene complexes)

IT 186692-55-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and coordinative substitution reactions with diphosphines)

IT 186692-56-8P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal structure of)

IT 167545-45-1P, (1,1'-Bis(diisopropylphosphino)ferrocene) (1,5-
cyclooctadiene) iridium(1+) tetraphenylborate

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT 186692-54-6P

RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT
(Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC
(Process); RACT (Reactant or reagent)

(preparation, crystal structure and kinetics of conformational inversion of)

IT 167545-42-8P, (1,1'-Bis(diisopropylphosphino)ferrocene) (1,5-
cyclooctadiene) iridium(1+) hexafluorophosphate

RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT
(Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC
(Process); RACT (Reactant or reagent)

(preparation, metathesis and kinetics of conformational inversion of)

RE.CNT 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD

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- (5) Broadwood-Strong, G; Polyhedron 1993, V12, P721 HCPLUS
- (6) Butler, I; Synth React Inorg Metal-Org Chem 1985, V15, P109 HCPLUS
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- (23) Sheldrick, G; SHELXL 93 1993
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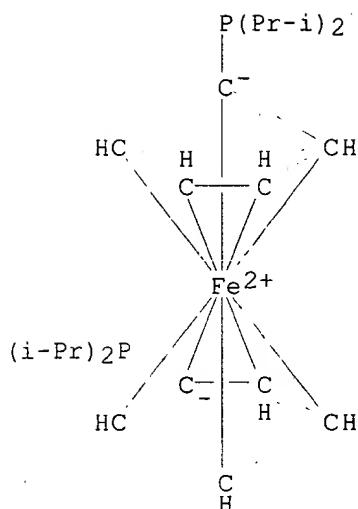
IT 97239-80-0, 1,1'-Bis(diisopropylphosphino)ferrocene

RL: RCT (Reactant); RACT (Reactant or reagent)

(coordinative substitution reactions with iridium and **rhodium**
diene complexes)

RN 97239-80-0 HCPLUS

CN Ferrocene, 1,1'-bis[bis(1-methylethyl)phosphino]- (9CI) (CA INDEX NAME)

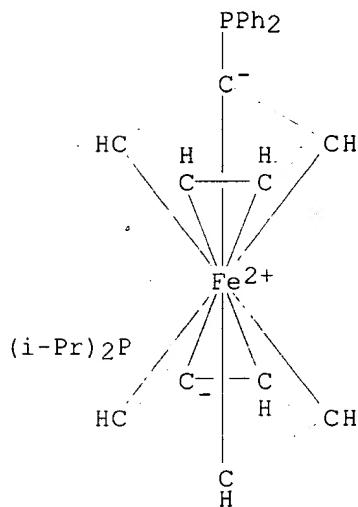


IT 97239-85-5, 1-Diisopropylphosphino-1'-diphenylphosphinoferrocene
 RL: RCT (Reactant); RACT (Reactant or reagent)

(coordinative substitution with iridium COD pyridine complex)

RN 97239-85-5 HCAPLUS

CN Ferrocene, 1-[bis(1-methylethyl)phosphino]-1'-(diphenylphosphino)- (9CI)
 (CA INDEX NAME)



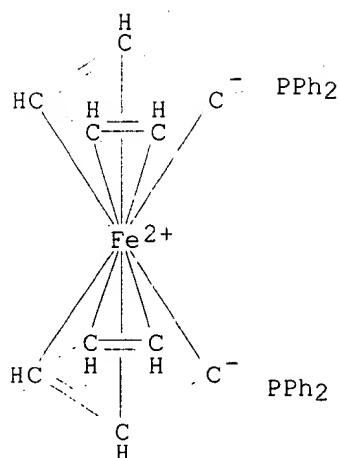
IT 12150-46-8, 1,1'-Bis(diphenylphosphino)ferrocene

RL: RCT (Reactant); RACT (Reactant or reagent)

(coordinative substitution with **rhodium**
 bis(diisopropylphosphino)ferrocene diene complex)

RN 12150-46-8 HCAPLUS

CN Ferrocene, 1,1'-bis(diphenylphosphino)- (9CI) (CA INDEX NAME)



IT 79790-98-0P, (1,1'-Bis(diphenylphosphino)ferrocene) (norbornadiene) rhodium(1+) tetrafluoroborate

RL: SPN (Synthetic preparation); PREP (Preparation)
(formation by coordinative substitution with
bis(diisopropylphosphino)ferrocene analog)

RN 79790-98-0 HCAPLUS

CN Rhodium(1+), [(2,3,5,6- η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis(diphenylphosphino- κ P)ferrocene]-, tetrafluoroborate(1-) (9CI)
(CA INDEX NAME)

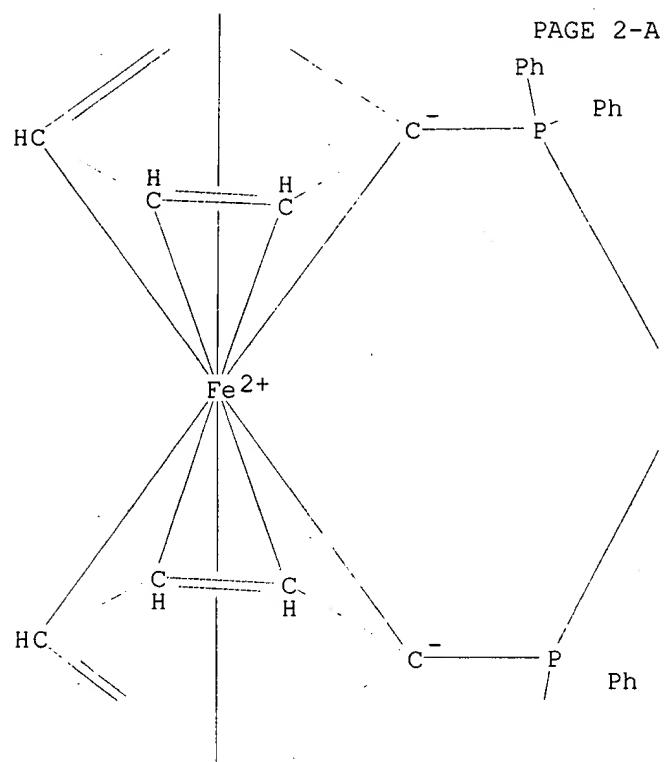
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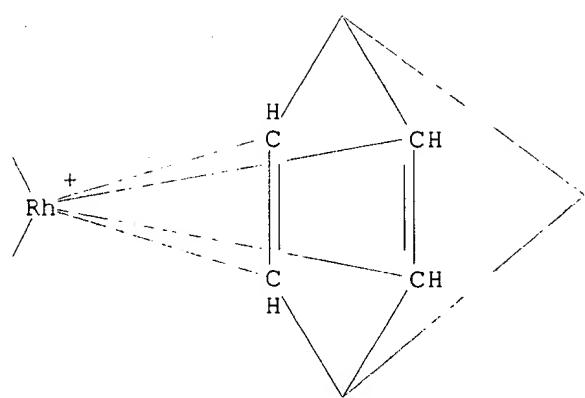
CMF C41 H36 Fe P2 Rh

CCI CCS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *



PAGE 2-B

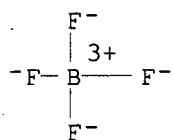


PAGE 3-A
Ph

C
H

CM 2

CRN 14874-70-5
CMF B F4
CCI CCS



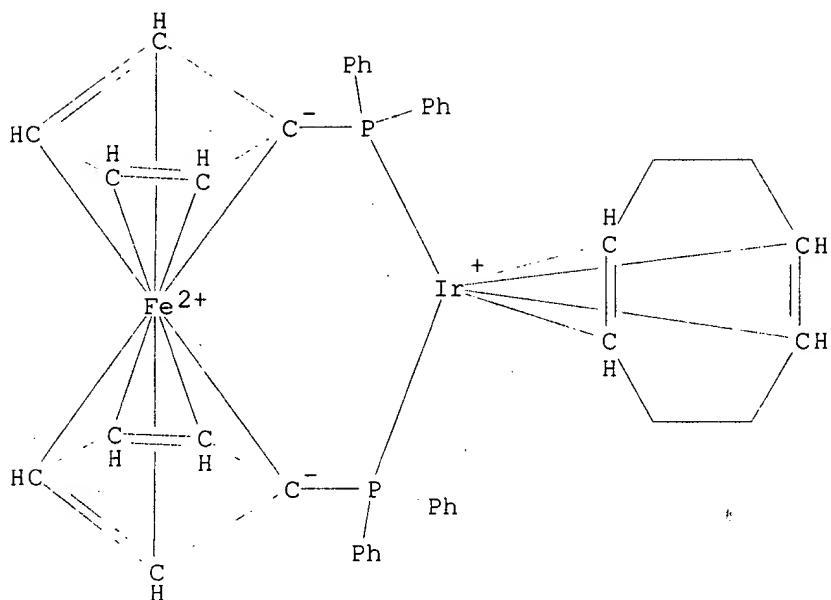
IT 151705-16-7, (1,1'-Bis(diphenylphosphino)ferrocene)(1,5-cyclooctadiene)iridium(1+) hexafluorophosphate
RL: PEP (Physical, engineering or chemical process); PRP (Properties);
PROC (Process)
(kinetics of conformational inversion and comparison to other
bisphosphinoferrocene complexes)

RN 151705-16-7 HCAPLUS

CN Iridium(1+), [1,1'-bis(diphenylphosphino- κ P)ferrocene][(1,2,5,6- η)-1,5-cyclooctadiene]-, hexafluorophosphate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 112947-50-9
CMF C42 H40 Fe Ir P2
CCI CCS

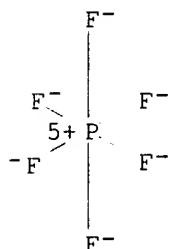


CM 2

CRN 16919-18-9

CMF F6 P

CCI CCS



IT 186692-55-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and coordinative substitution reactions with diphosphines)

RN 186692-55-7 HCAPLUS

CN Rhodium(1+), [(2,3,5,6- η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis[bis(1-methylethyl)phosphino- κP]ferrocene]-, tetrafluoroborate(1-)
(9CI) (CA INDEX NAME)

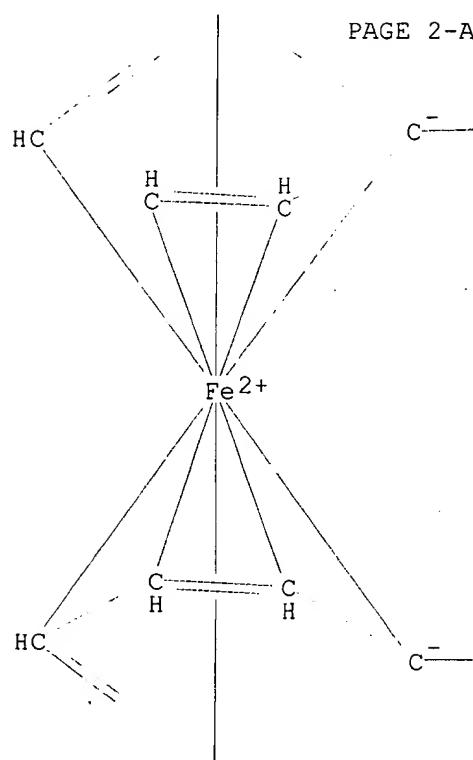
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CRN 96144-62-6

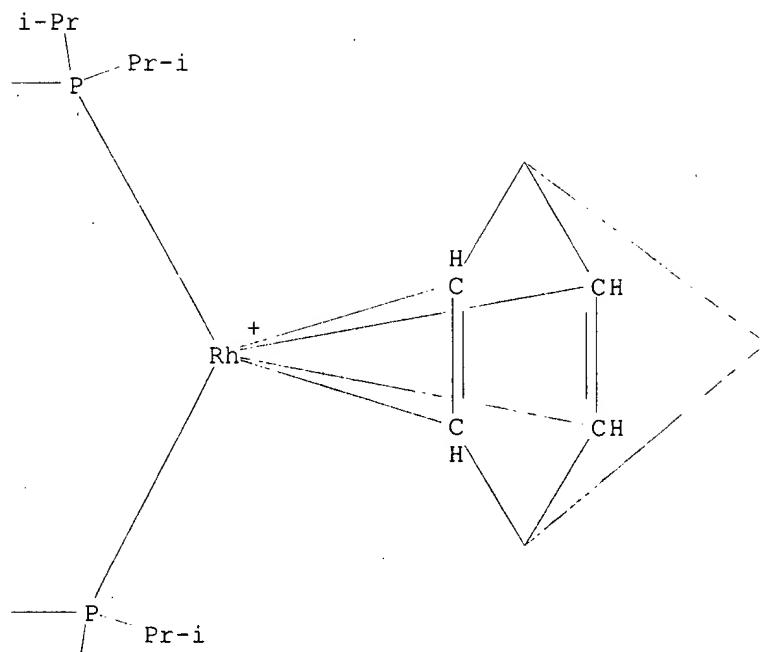
CMF C29 H44 Fe P2 Rh

CCI CCS

PAGE 2-A



PAGE 2-B



PAGE 3-A

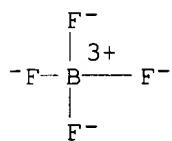
C
H

PAGE 3-B

i-Pr

CM 2

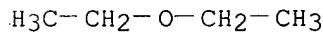
CRN 14874-70-5
 CMF B F4
 CCI CCS



IT 186692-56-8P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (preparation and crystal structure of)
 RN 186692-56-8 HCPLUS
 CN Rhodium(1+), [(2,3,5,6- η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-
 bis[bis(1-methylethyl)phosphino- κ P]ferrocene]-, tetrafluoroborate(1-
), compd. with 1,1'-oxybis[ethane] (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 60-29-7
 CMF C4 H10 O



CM 2

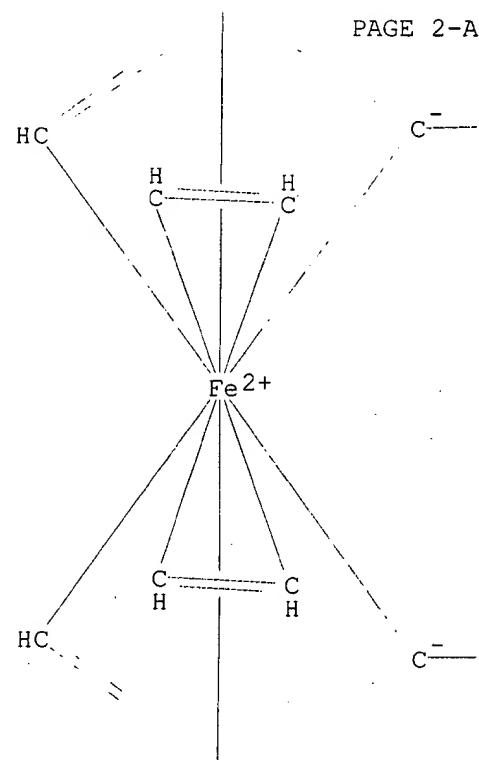
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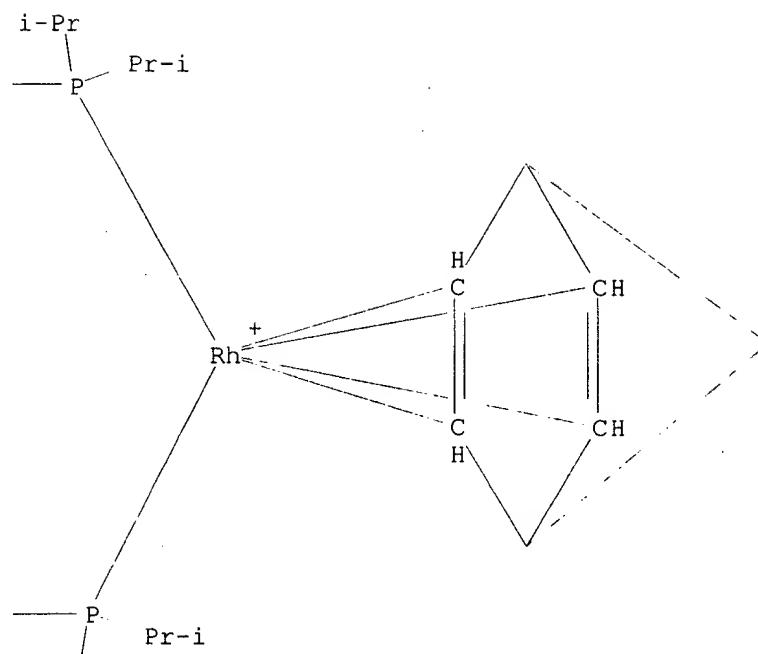
CRN 96144-62-6
 CMF C29 H44 Fe P2 Rh
 CCI CCS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



PAGE 2-B



PAGE 3-A

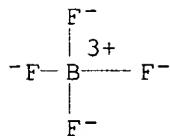
C
H

PAGE 3-B

i-Pr

CM 4

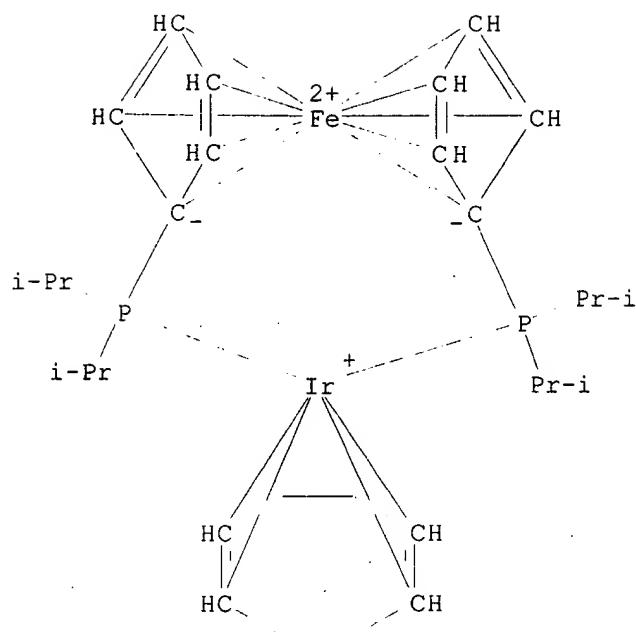
CRN 14874-70-5
 CMF B F4
 CCI CCS



IT 167545-45-1P, (1,1'-Bis(diisopropylphosphino)ferrocene)(1,5-cyclooctadiene)iridium(1+) tetraphenylborate
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 167545-45-1 HCPLUS
 CN Iridium(1+), [1,1'-bis[bis(1-methylethyl)phosphino-
 κP]ferrocene][(1,2,5,6-η)-1,5-cyclooctadiene]-,
 tetraphenylborate(1-) (9CI) (CA INDEX NAME)

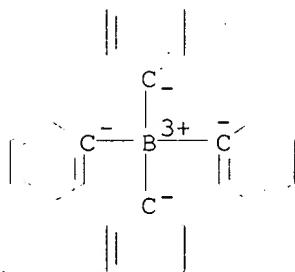
CM 1

CRN 167545-41-7
 CMF C30 H48 Fe Ir P2
 CCI CCS



CM 2

CRN 4358-26-3
 CMF C24 H20 B
 CCI CCS



IT 186692-54-6P

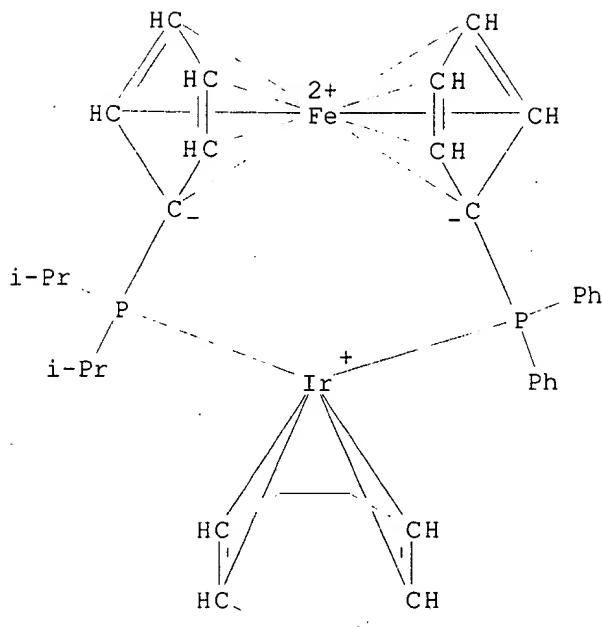
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
 (preparation, crystal structure and kinetics of conformational inversion of)

RN 186692-54-6 HCPLUS

CN Iridium(1+), [1-[bis(1-methylethyl)phosphino-κP]-1'-(diphenylphosphino-κP)ferrocene][(1,2,5,6-η)-1,5-cyclooctadiene]-, hexafluorophosphate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 186692-53-5
 CMF C36 H44 Fe Ir P2
 CCI CCS

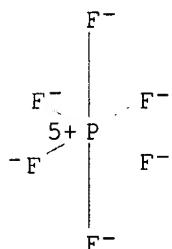


CM 2

CRN 16919-18-9

CMF F6 P

CCI CCS



IT 167545-42-8P, (1,1'-Bis(diisopropylphosphino)ferrocene)(1,5-cyclooctadiene)iridium(1+) hexafluorophosphate

RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)

(preparation, metathesis and kinetics of conformational inversion of)

RN 167545-42-8 HCPLUS

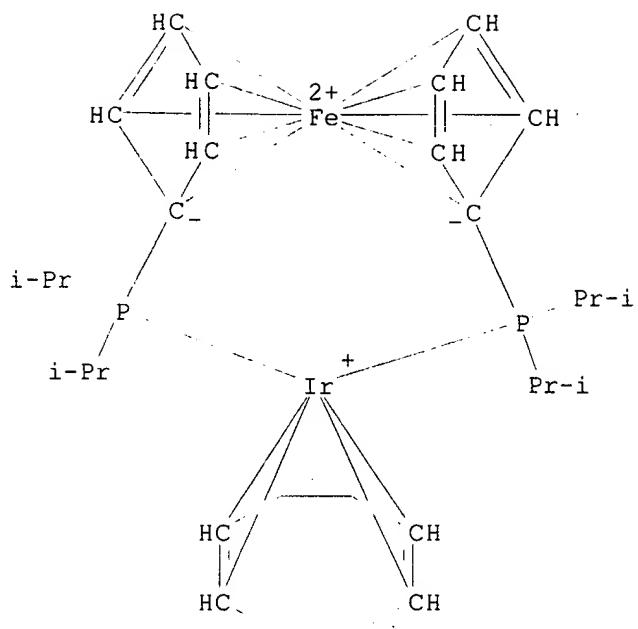
CN Iridium(1+), [1,1'-bis[bis(1-methylethyl)phosphino- κ P]ferrocene][(1,2,5,6- η)-1,5-cyclooctadiene]-, hexafluorophosphate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 167545-41-7

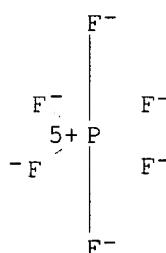
CMF C30 H48 Fe Ir P2

CCI CCS



CM 2

CRN 16919-18-9
 CMF F6 P
 CCI CCS



L104 ANSWER 9 OF 20 HCPLUS COPYRIGHT 2004 ACS on STN
 AN 1995:1004413 HCPLUS
 DN 124:116619
 ED Entered STN: 26 Dec 1995
 TI Catalytic cyclization of some alkynes by rhodium and iridium complexes of ferrocene-containing ligands
 AU Kim, Tae-Jeong; Kim, So-Hoon; Shim, Sang-Chul; Jeong, Jong-Hwa
 CS Dep. of Industrial Chemistry, Kyungpook National Univ., Taegu, 702-701, S. Korea
 SO Bulletin of the Korean Chemical Society (1995), 16(11), 1126-8
 CODEN: BKCSDE; ISSN: 0253-2964
 PB Korean Chemical Society
 DT Journal
 LA English

CC 23-4 (Aliphatic Compounds)
Section cross-reference(s): 29, 75

OS CASREACT 124:116619

AB The lactonization of 4-pentyoic acid and the cocyclotrimerization of N-benzylpropargylamine with PhC.tplbond.CH, both reaction catalyzed by Rh and Ir complexes with ferrocenylphosphines and -imines, were studied. [(COD)Ir(PPFA)]ClO₄ (PPFA = 2-diphenylphosphino-1-(N,N-dimethylaminoethyl)ferrocene) was prepared and its crystal structure determined

ST crystal structure iridium aminoethylphosphinoferrocene; aminoethylphosphinoferrocene iridium prepn structure; cyclization catalyst iridium rhodium phosphinoferrocene alkyne

IT Alkynes
RL: RCT (Reactant); RACT (Reactant or reagent)
(catalytic cyclization in presence of iridium and rhodium phosphinoferrocene complexes)

IT Ring closure catalysts
(iridium and rhodium phosphinoferrocene complexes for alkynes)

IT 536-74-3, Phenylacetylene 1197-51-9 6089-09-4, 4-Pentyoic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(catalytic cyclization in presence of iridium and rhodium phosphinoferrocene complexes)

IT 91159-10-3 112947-51-0 **125939-72-2** 173101-24-1 173101-26-3
173101-28-5 173967-26-5
RL: CAT (Catalyst use); USES (Uses)
(cyclization catalysts for alkynes)

IT 12112-67-3, Dichlorobis(cyclooctadiene)diiridium 105088-01-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(for preparation of iridium cyclooctadiene aminoethylphosphinoferrocene complex)

IT 173101-31-0P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal structure of)

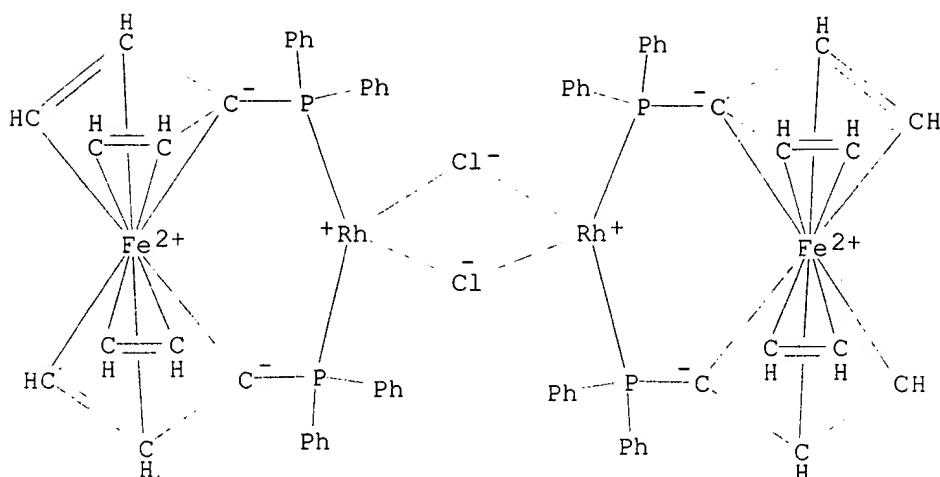
IT 173101-30-9P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and mol. structure of)

IT 10008-73-8P 173101-22-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation by catalytic cyclization of alkynes in presence of iridium and rhodium phosphinoferrocene complexes)

IT **125939-72-2**
RL: CAT (Catalyst use); USES (Uses)
(cyclization catalysts for alkynes)

RN 125939-72-2 HCPLUS

CN Rhodium, bis[1,1'-bis(diphenylphosphino)ferrocene-P,P']di- μ -chlorodi- (9CI) (CA INDEX NAME)



L104 ANSWER 10 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1994:578803 HCAPLUS

DN 121:178803

ED Entered STN: 15 Oct 1994

TI Efficient rhodium-catalyzed hydrogenation of aldehydes and ketones

AU Burk, Mark J.; Harper, T. Gregory P.; Lee, Jeffrey R.; Kalberg, Christopher

CS Dep. Chem., Duke Univ., Durham, NC, 27706, USA

SO Tetrahedron Letters (1994), 35(28), 4963-6

CODEN: TELEAY; ISSN: 0040-4039

DT Journal

LA English

CC 21-2 (General Organic Chemistry)

OS CASREACT 121:178803

AB A cationic rhodium(I) catalyst bearing the air-stable and crystalline diphosphine 1,1'-bis(diisopropylphosphino)ferrocene allows the hydrogenation of aldehydes and ketones under mild conditions.

ST rhodium ferrocene catalyst hydrogenation carbonyl; aldehyde hydrogenation rhodium catalyst; ketone hydrogenation rhodium catalyst

IT Aldehydes, reactions

Ketones, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrogenation of, rhodium ferrocene complex as catalyst for)

IT Hydrogenation catalysts

(rhodium ferrocene complex, for aldehydes and ketones)

IT 97239-80-0

RL: CAT (Catalyst use); USES (Uses)
(catalysts, containing bis(cyclooctadiene)rhodium triflate, for hydrogenation of aldehydes and ketones)

IT 99326-34-8

RL: CAT (Catalyst use); USES (Uses)
(catalysts, containing bis(diisopropylphosphino)ferrocene, for hydrogenation of aldehydes and ketones)

IT 157772-66-2

RL: CAT (Catalyst use); USES (Uses)
(catalysts, for hydrogenation of aldehydes and ketones)

IT 66-25-1, Hexanal 78-93-3, 2-Butanone, reactions 98-01-1
, 2-Furancarboxaldehyde, reactions 98-03-3, 2-
Thiophenecarboxaldehyde 98-53-3 98-86-2, Acetophenone,
reactions 100-52-7, Benzaldehyde, reactions
108-94-1, Cyclohexanone, reactions 119-53-9, Benzoin 122-57-6,
Benzalacetone 372-31-6 434-45-7, Trifluoroacetophenone 513-86-0
609-38-1, 2-Furancarboxamide 630-19-3, Pivalaldehyde
1603-79-8, Ethyl oxophenylacetate 1694-31-1, tert-Butyl 3-oxobutanoate
3524-62-7 3891-59-6 7152-15-0, Pentanoic acid, 4-methyl-3-oxo-, ethyl
ester 20201-24-5, Butanoic acid, 3-methyl-2-oxo-, ethyl ester
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrogenation of, rhodium ferrocene complex as
catalyst for)

IT 2550-26-7P, 4-Phenyl-2-butanone
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and hydrogenation of, rhodium ferrocene
complex as catalyst for)

IT 2344-70-9P, 4-Phenyl-2-butanol
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT 100-51-6P, Benzyl alcohol, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by rhodium complex-catalyzed
hydrogenation of benzaldehyde)

IT 579-43-1P 655-48-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by rhodium complex-catalyzed
hydrogenation of benzoin)

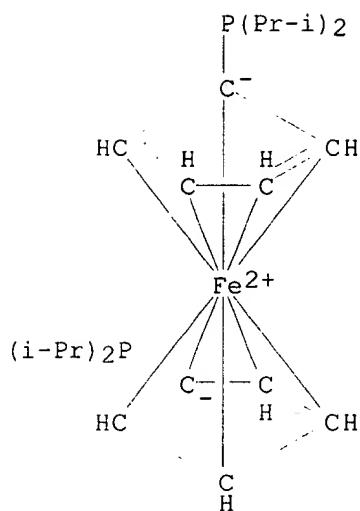
IT 5341-95-7P 6982-25-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by rhodium complex-catalyzed
hydrogenation of hydroxybutanone)

IT 937-05-3P, Cyclohexanol, 4-(1,1-dimethylethyl)-, cis- 21862-63-5P,
Cyclohexanol, 4-(1,1-dimethylethyl)-, trans-
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by rhodium complex-catalyzed
hydrogenation of ketone)

IT 97239-80-0
RL: CAT (Catalyst use); USES (Uses)
(catalysts, containing bis(cyclooctadiene)rhodium triflate, for
hydrogenation of aldehydes and ketones)

RN 97239-80-0 HCPLUS

CN Ferrocene, 1,1'-bis[bis(1-methylethyl)phosphino]- (9CI) (CA INDEX NAME)



IT 157772-66-2

RL: CAT (Catalyst use); USES (Uses)
 (catalysts, for **hydrogenation of aldehydes and ketones**)

RN 157772-66-2 HCAPLUS

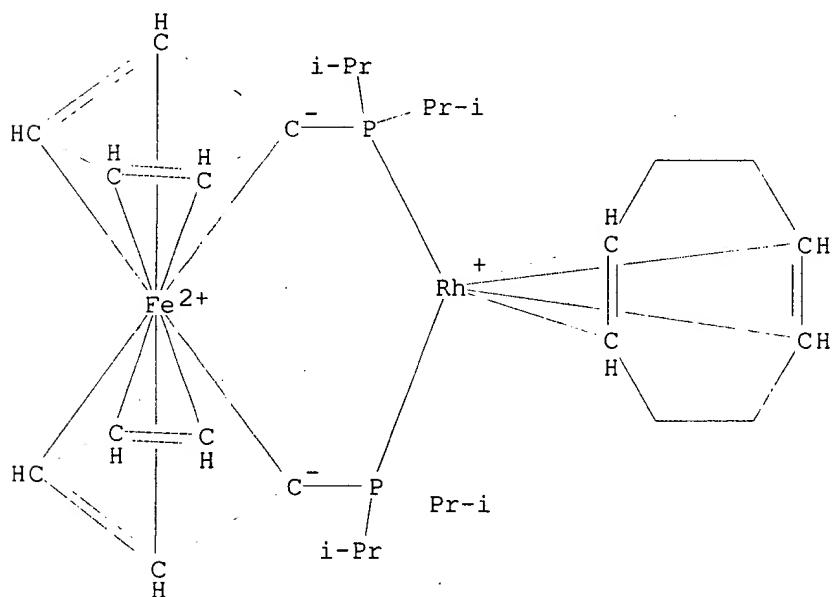
CN Rhodium(1+), [1,1'-bis[bis(1-methylethyl)phosphino]ferrocene-
 P,P'][(1,2,5,6-η)-1,5-cyclooctadiene]-, salt with
 trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 157772-65-1

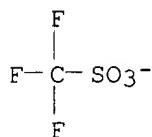
CMF C30 H48 Fe P2 Rh

CCI CCS

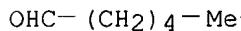


CM 2

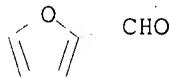
CRN 37181-39-8
 CMF C F3 O3 S



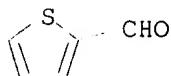
IT 66-25-1, Hexanal 98-01-1, 2-Furancarboxaldehyde
 , reactions 98-03-3, 2-Thiophenecarboxaldehyde
 100-52-7, Benzaldehyde, reactions 630-19-3,
 Pivalaldehyde
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (hydrogenation of, rhodium ferrocene complex as
 catalyst for)
 RN 66-25-1 HCAPLUS
 CN Hexanal (8CI, 9CI) (CA INDEX NAME)



RN 98-01-1 HCAPLUS
 CN 2-Furancarboxaldehyde (9CI) (CA INDEX NAME)



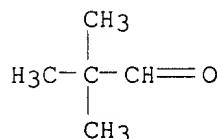
RN 98-03-3 HCAPLUS
 CN 2-Thiophenecarboxaldehyde (7CI, 8CI, 9CI) (CA INDEX NAME)



RN 100-52-7 HCAPLUS
 CN Benzaldehyde (7CI, 8CI, 9CI) (CA INDEX NAME)



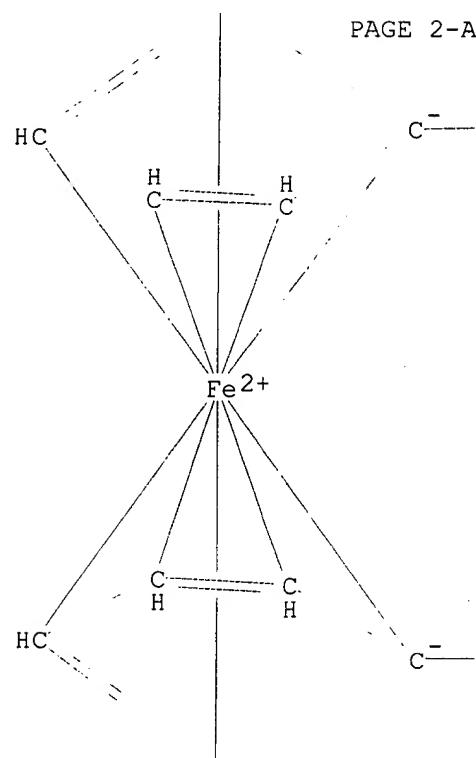
RN 630-19-3 HCAPLUS
 CN Propanal, 2,2-dimethyl- (9CI) (CA INDEX NAME)



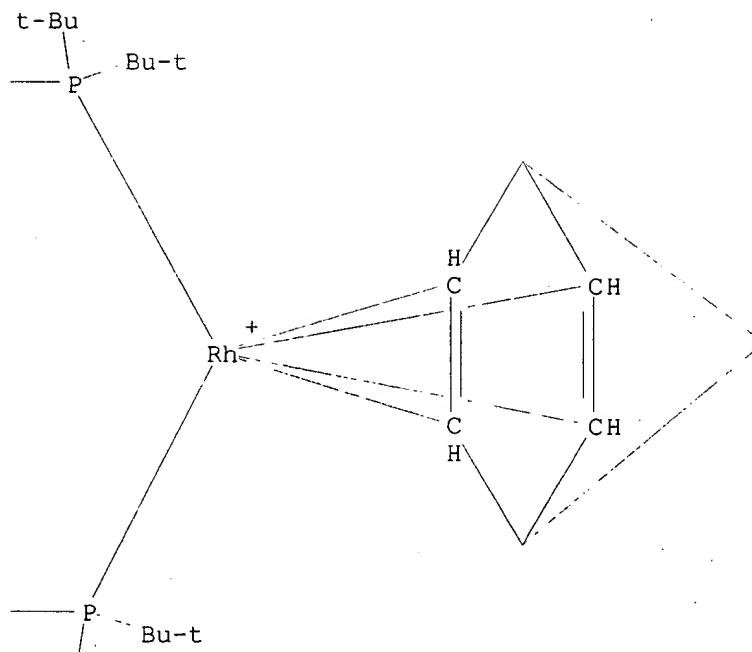
L104 ANSWER 11 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1990:603799 HCAPLUS
DN 113:203799
ED Entered STN: 23 Nov 1990
TI Synthesis and solution chemistry of metal hydrides from cationic
rhodium(I) catalyst precursors $[(L-L)Rh(NBD)ClO_4]$ ($L-L =$
 $Fe(\eta^5-C_5H_4PBu-tert)_2$, $Fe(\eta^5-C_5H_4PPhBu-tert)_2$)
AU Kim, Tae Jeong
CS Dep. Ind. Chem., Kyungpook Natl. Univ., Taegu, 702-701, S. Korea
SO Bulletin of the Korean Chemical Society (1990), 11(2), 134-9
CODEN: BKCSDE; ISSN: 0253-2964
DT Journal
LA English
CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 29, 77
AB The **hydrogenation** catalyst precursors $[(L-L)Rh$
 $(NBD)ClO_4$ ($L-L = Fe(\eta^5-C_5H_4P(CMe_3)_2)_2$, $Fe(\eta^5-C_5H_4PPhCMe_3)_2$; NBD =
norbornadiene) react with H₂ (1 atm, 30°, MeOH) to yield
 $[(L-L)HRh(\mu-H)_3RhH(L-L)]ClO_4$. These hydrido species are fluxional, and
variable temperature NMR studies show the existence of a number of equilibrium
involving
both fluxional and nonfluxional species. The synthesis, solution structures,
and fluxional behaviors of these hydrides are described.
ST fluxionality **rhodium** hydrido ferrocenylphosphine dinuclear;
phosphine ferrocenyl **rhodium** hydrido dinuclear
IT Fluxional rearrangement
(of **rhodium** hydrido ferrocenylphosphine dinuclear complexes)
IT 84680-97-7 92284-06-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrogenation of)
IT 92468-70-7P 130322-22-4P
RL: PEP (Physical, engineering or chemical process); RCT (Reactant); SPN
(Synthetic preparation); PREP (Preparation); PROC (Process); RACT
(Reactant or reagent)
(preparation and fluxionalty of)
IT 84680-97-7 92284-06-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrogenation of)
RN 84680-97-7 HCAPLUS
CN Rhodium(1+), [(2,3,5,6- η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-
bis[bis(1,1-dimethylethyl)phosphino]ferrocene-P,P']- (9CI) (CA INDEX
NAME)

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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H

PAGE 3-B

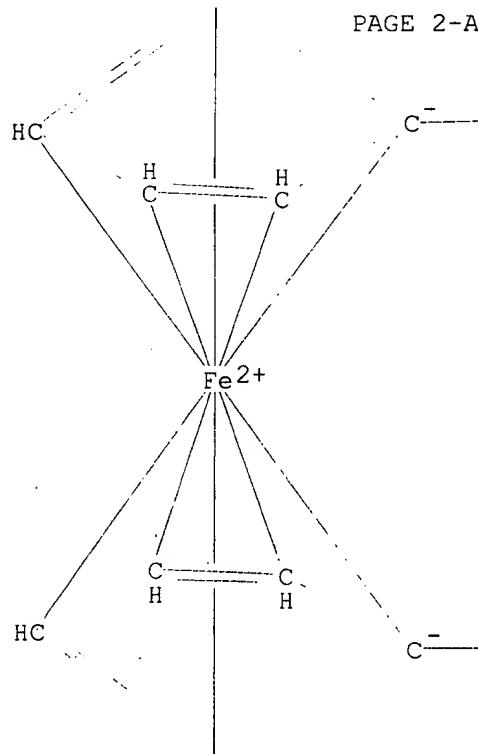
t-Bu

RN 92284-06-5 HCPLUS

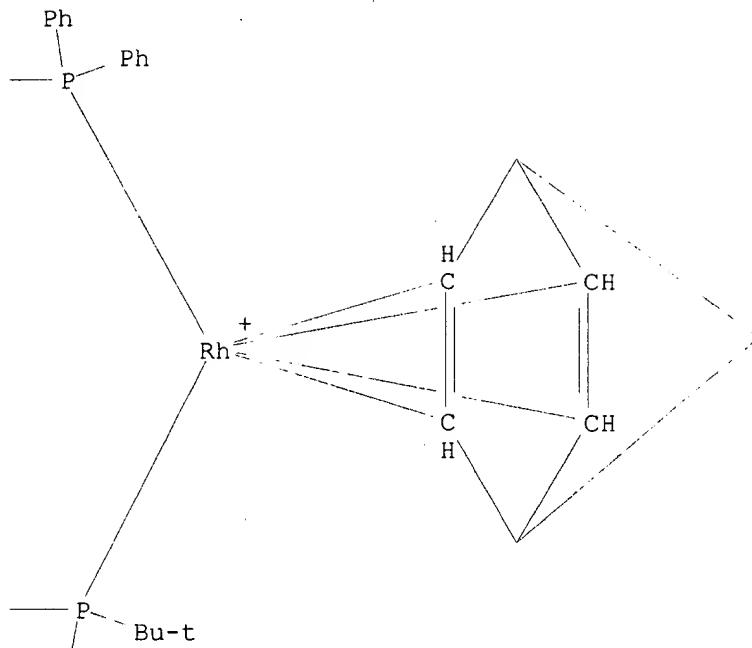
CN Rhodium(1+), [(2,3,5,6- η)-bicyclo[2.2.1]hepta-2,5-diene][1-[bis(1,1-dimethylethyl)phosphino]-1'-(diphenylphosphino)ferrocene-P,P']- (9CI) (CA INDEX NAME)

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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PAGE 3-A



PAGE 3-B

t-Bu

IT 92468-70-7P 130322-22-4P

RL: PEP (Physical, engineering or chemical process); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
(preparation and fluxionality of)

RN 92468-70-7 HCAPLUS

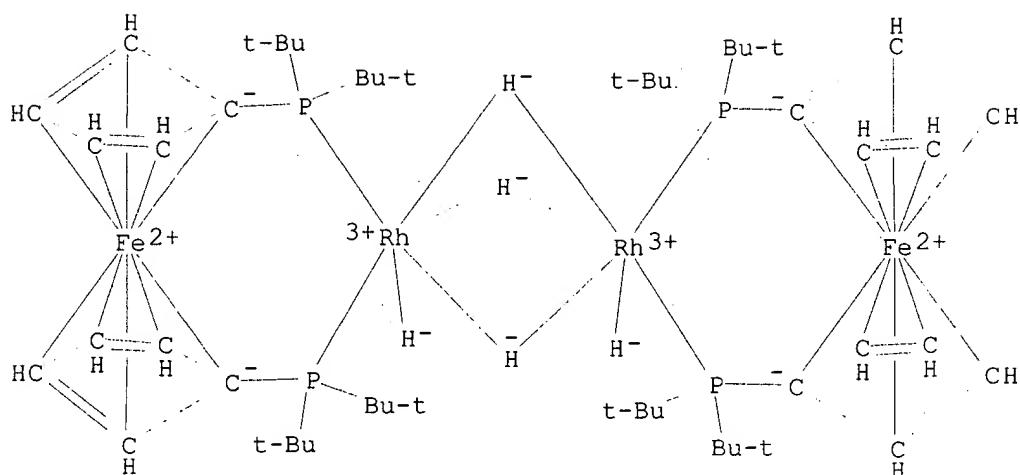
CN Rhodium(1+), bis[1,1'-bis[bis(1,1-dimethylethyl)phosphino]ferrocene-P,P']tri-μ-hydrodihydrodi-, perchlorate (9CI) (CA INDEX NAME)

CM 1

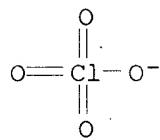
CRN 92468-69-4

CMF C52 H93 Fe2 P4 Rh2

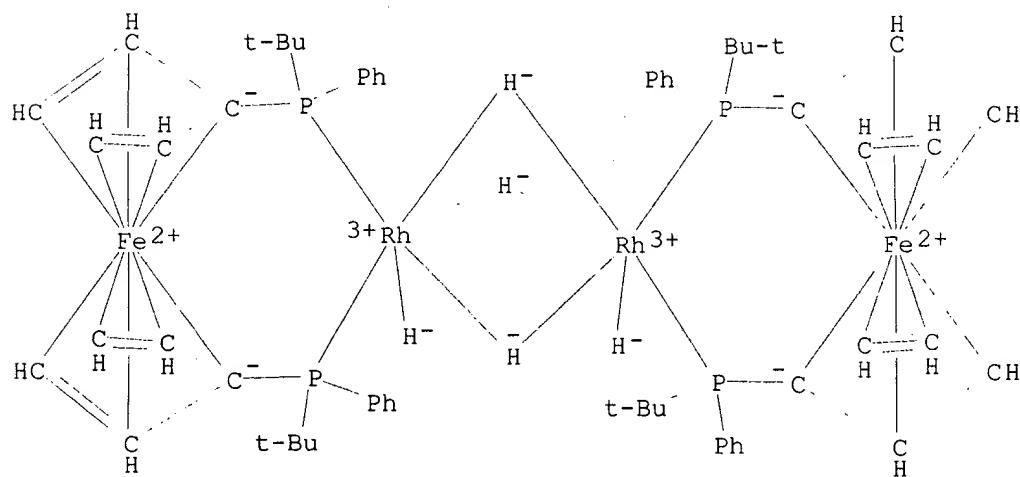
CCI CCS



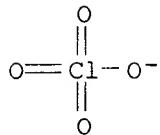
CM 2

CRN 14797-73-0
CMF Cl O4RN 130322-22-4 HCPLUS
CN Rhodium(1+), bis[1,1'-bis[(1,1-dimethylethyl)phenylphosphino]ferrocene-P,P']tri- μ -hydrodihydrodi-, perchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 130322-21-3
CMF C60 H77 Fe2 P4 Rh2
CCI CCS

CM 2

CRN 14797-73-0
CMF Cl O4

L104 ANSWER 12 OF 20 HCPLUS COPYRIGHT 2004 ACS on STN
 AN 1990:139478 HCPLUS
 DN 112:139478
 ED Entered STN: 13 Apr 1990
 TI Rhodium(I) complexes of 1,1'-bis(diphenylphosphino)ferrocene as efficient catalysts in regioselective hydrogenation of polynuclear heteroaromatic compounds
 AU Kim, Tae Jeong; Lee, Kyu Chul
 CS Dep. Ind. Chem., Kyungpook Natl. Univ., Taegu, 702-701, S. Korea
 SO Bulletin of the Korean Chemical Society (1989), 10(3), 279-82
 CODEN: BKCSDE; ISSN: 0253-2964
 DT Journal
 LA English
 CC 29-13 (Organometallic and Organometalloidal Compounds)
 Section cross-reference(s): 22, 27
 AB Two rhodium(I) complexes of the types [Rh(BPPF)(NBD)]ClO4 (I) and [Rh(BPPF)Cl]2 (II) (BPPF = 1,1'-bis(diphenylphosphino)ferrocene, NBD = norbornadiene) were prepared and investigated as catalysts for the regioselective hydrogenation of polynuclear heteroarom. N and S compds. such as quinoline, acridine, phenanthridine, 7,8-benzoquinoline, benzothiophene, isoquinoline, indole, pyridine, and thiophene. Both complexes I and II, except for the cases of indole and mononuclear heteroaroms. pyridine and thiophene, are very efficient in the selective reduction under quite mild hydrogenation conditions to give the corresponding saturated N and S heterocyclic analogs in fast conversion rates and in excellent yields. Relative rate studies revealed that the reduction depends significantly on the steric and electronic effects of the substrates. Of the two complexes, the dimeric species II gives faster reaction rates in all cases studied.
 ST phenylphosphinoferrocene rhodium complex regioselective hydrogenation catalyst; heterocyclic nitrogen sulfur hydrogenation catalyst; kinetics hydrogenation nitrogen sulfur heterocycle
 IT Hydrogenation catalysts
 (bis(diphenylphosphino)ferrocene rhodium complexes, for nitrogen and sulfur heterocycles)
 IT Regiochemistry
 (of hydrogenation of nitrogen and sulfur heterocycles, rhodium complex-catalyzed)
 IT Kinetics of hydrogenation
 (of nitrogen and sulfur heterocyclic compds., rhodium -catalyzed)
 IT Heterocyclic compounds
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (nitrogen, regioselective hydrogenation of, rhodium catalysts for)
 IT Heterocyclic compounds
 RL: RCT (Reactant); RACT (Reactant or reagent)

(sulfur, regioselective hydrogenation of, **rhodium** catalysts for)

IT 110-02-1, Thiophene 110-86-1, Pyridine, reactions 120-72-9, 1H-Indole, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (attempted hydrogenation of, **rhodium**-catalyzed)

IT **84680-96-6**
 RL: CAT (Catalyst use); USES (Uses)
 (catalyst, for regioselective hydrogenation of nitrogen and sulfur heterocycles)

IT 7727-37-9
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (heterocyclic compounds, nitrogen, regioselective hydrogenation of, **rhodium** catalysts for)

IT 7704-34-9
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (heterocyclic compounds, sulfur, regioselective hydrogenation of, **rhodium** catalysts for)

IT 91-22-5, Quinoline, reactions 95-15-8, Benzothiophene 119-65-3, Isoquinoline 229-87-8, Phenanthridine 230-27-3, 7,8-Benzoquinoline 260-94-6, Acridine
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (hydrogenation of, (diphenylphosphino)**ferrocene****rhodium** complex catalysts for, regiochem. and kinetics of)

IT **125939-72-2**
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation as hydrogenation catalyst, for nitrogen and sulfur heterocycles)

IT 91-21-4P 92-81-9P 635-46-1P 4565-32-6P 5223-80-3P 27799-79-7P
125916-39-4P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

IT **12150-46-8**
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (substitution reaction by, of norbornadiene **rhodium** complex)

IT 12257-42-0
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (substitution reaction of, with bis(diphenylphosphino)ferrocene)

IT **84680-96-6**
 RL: CAT (Catalyst use); USES (Uses)
 (catalyst, for regioselective hydrogenation of nitrogen and sulfur heterocycles)

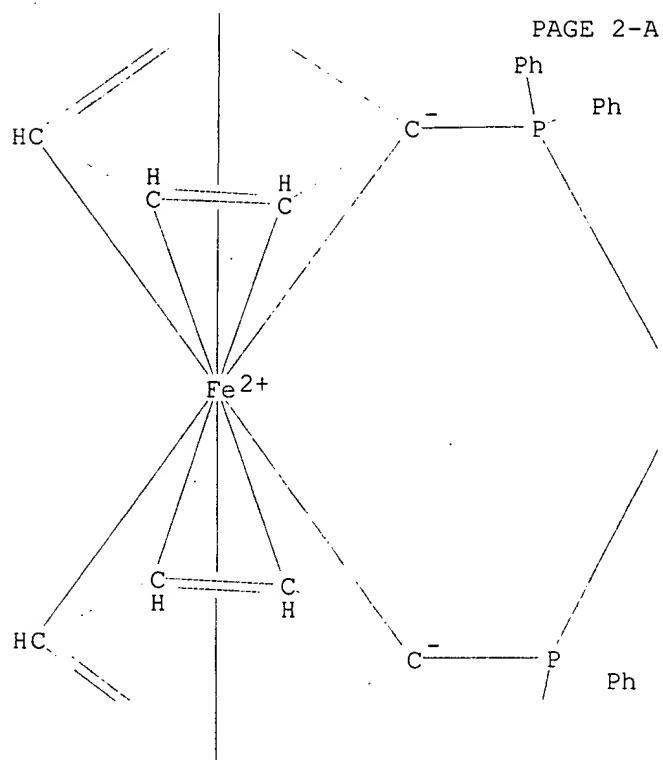
RN 84680-96-6 HCAPLUS

CN Rhodium(1+), [(2,3,5,6- η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis(diphenylphosphino- κ P)ferrocene]-, perchlorate (9CI) (CA INDEX NAME)

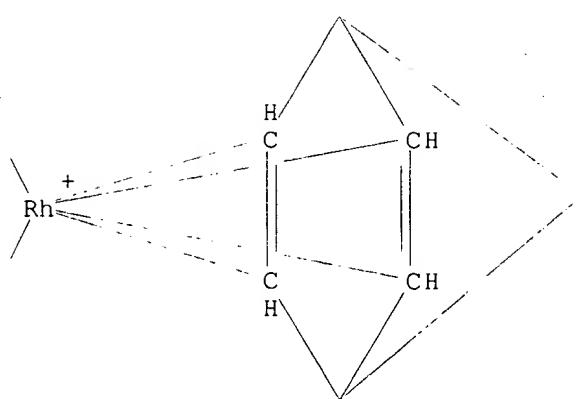
CM 1

CRN 79790-97-9
 CMF C41 H36 Fe P2 Rh
 CCI CCS

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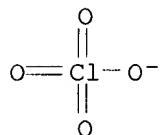


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PAGE 3-A
Ph

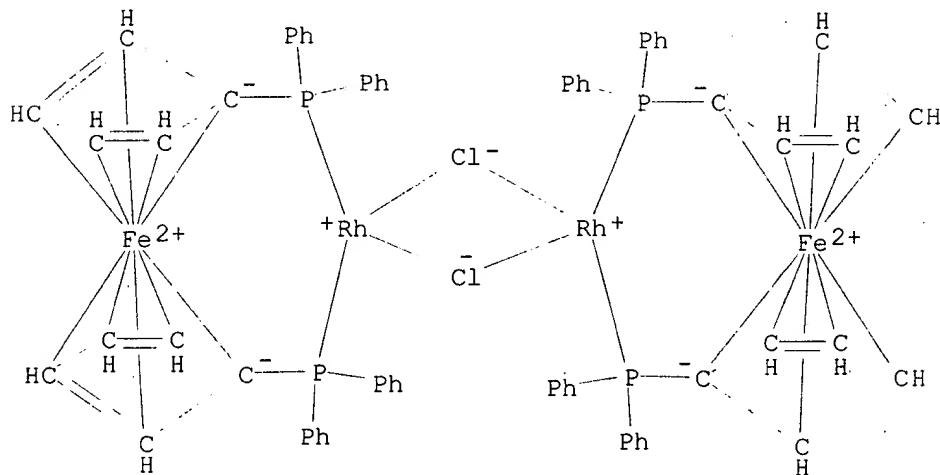
CM 2

CRN 14797-73-0
CMF C1 O4

IT 125939-72-2

RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation as hydrogenation catalyst, for nitrogen and sulfur heterocycles)

RN 125939-72-2 HCPLUS

CN Rhodium, bis[1,1'-bis(diphenylphosphino)ferrocene-P,P']di- μ -chlorodi- (9CI) (CA INDEX NAME)

IT 125916-39-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

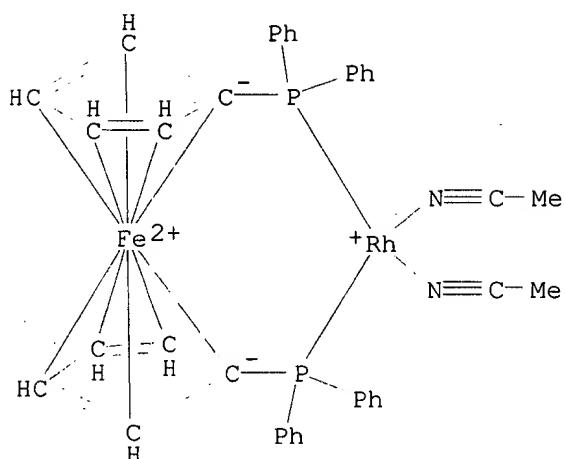
RN 125916-39-4 HCPLUS

CN Rhodium(1+), bis(acetonitrile)[1,1'-bis(diphenylphosphino)ferrocene-P,P']- (SP-4-2)-, perchlorate (9CI) (CA INDEX NAME)

CM 1

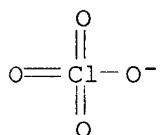
CRN 125916-38-3

CMF C38 H34 Fe N2 P2 Rh
CCI CCS



CM 2

CRN 14797-73-0
CMF Cl O4

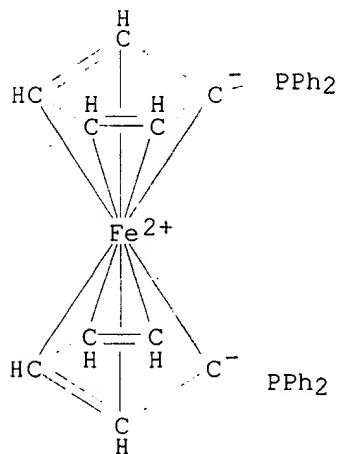


IT 12150-46-8

RL: RCT (Reactant); RACT (Reactant or reagent)
(substitution reaction by, of norbornadiene rhodium complex)

RN 12150-46-8 HCPLUS

CN Ferrocene, 1,1'-bis(diphenylphosphino)- (9CI) (CA INDEX NAME)



AN 1985:471462 HCAPLUS
 DN 103:71462
 ED Entered STN: 07 Sep 1985
 TI 1,1'-Bis(alkylarylphosphino)ferrocenes: synthesis, metal complex formation, and crystal structure of three metal complexes of $\text{Fe}(\eta^5\text{-C}_5\text{H}_4\text{PPh}_2)_2$
 AU Butler, Ian R.; Cullen, William R.; Kim, Tae Jeong; Rettig, Steven J.; Trotter, James
 CS Chem. Dep., Univ. British Columbia, Vancouver, BC, V6T 1Y6, Can.
 SO Organometallics (1985), 4(6), 972-80
 CODEN: ORGND7; ISSN: 0276-7333
 DT Journal
 LA English
 CC 29-12 (Organometallic and Organometalloidal Compounds)
 Section cross-reference(s): 75
 OS CASREACT 103:71462
 GI For diagram(s), see printed CA Issue.
 AB The ferrocenylbisphosphines I (R = PR₂R₃; R₁ = PR₄R₅) (R₂-R₅ = Ph or Me₃C) were prepared by treating either dilithio I (R = R₁ = Li) or I (R = Li, R₁ = PR₄R₅ (II) with Cl₂PR₂R₃. II was obtained by cleaving ferrocenophane I (RR₁ = PR₄) with R₅Li. Best results were obtained when R₄ and/or R₅ = Ph. A range of PdLC₁₂, NiLX₂, and [Rh(L)(NBD)]ClO₄ [L = I; R₁, R₂ = PPh₂, P(CMe₃)₂, PPhCMe₃; NBD = norbornadiene; X = Cl, Br] complexes were prepared. The crystal structures of PdLC₁₂, NiLBr₂, and MoL(CO)₄ (L = I; R = R₁ = PPh₂) showed the metal atoms had cis-square planar, tetrahedral, and cis-octahedral coordination, resp. The I (R = R₁ = PPh₂) ligands have slightly nonparallel cyclopentadienyl rings, with approx. staggered arrangements in the Pd and Mo compds. but an approx. eclipsed conformation in the Ni complex, with significant displacements of the P atoms from the ring planes. ML(CO)₄ (M = Mo, Cr; L = I; R = R₁ = PPh₂) are fluxional in solution to -80°.
 ST crystal structure ferrocenyl bisphosphine metal complex; mol structure ferrocenyl bisphosphine metal complex; phosphinoferrocene metal complex crystal structure; molybdenum bisphosphinoferrocene complex crystal structure; palladium bisphosphinoferrocene complex crystal structure; nickel bisphosphinoferrocene complex crystal structure; fluxionality chromium molybdenum bisphosphinoferrocene complex
 IT Crystal structure
 Molecular structure
 (of bisphosphinoferrocene metal complexes)
 IT Fluxional rearrangement
 (of chromium or molybdenum bisphosphinoferrocene complexes)
 IT 95408-44-9
 RL: PRP (Properties)
 (crystal structure of)
 IT 67292-28-8
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (fluxionality and mol. structure of)
 IT 67292-31-3
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (fluxionality of)
 IT 83547-83-5
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (lithiation and reaction of, with chlorophosphines)
 IT 72954-06-4
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (lithiation and reactions of, with chlorophosphine)
 IT 67292-33-5P 95464-05-4P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (preparation and crystal structure of)
 IT 72287-26-4P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (preparation and mol. structure of)

IT 95408-39-2P 95408-40-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and reaction of, with metal complex)

IT 95408-38-1P 95464-04-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and reactions of, with metal complexes)

IT 12098-17-8P 92269-95-9P 92284-07-6P 95408-41-6P
95408-42-7P 95408-45-0P 95408-46-1P 95408-47-2P 95408-48-3P
95408-49-4P 95408-51-8P 95408-52-9P 95420-22-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT 1079-66-9 13716-10-4 29949-69-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, for lithiated phosphinoferrocene)

IT 10025-98-6 12107-56-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with bisphosphinoferrocene complexes)

IT 95408-37-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with chlorophosphine)

IT 12150-46-8 84680-95-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with palladium or nickel complex)

IT 14220-64-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactions of, with bisphosphinoferrocene complexes)

IT 92269-95-9P 92284-07-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

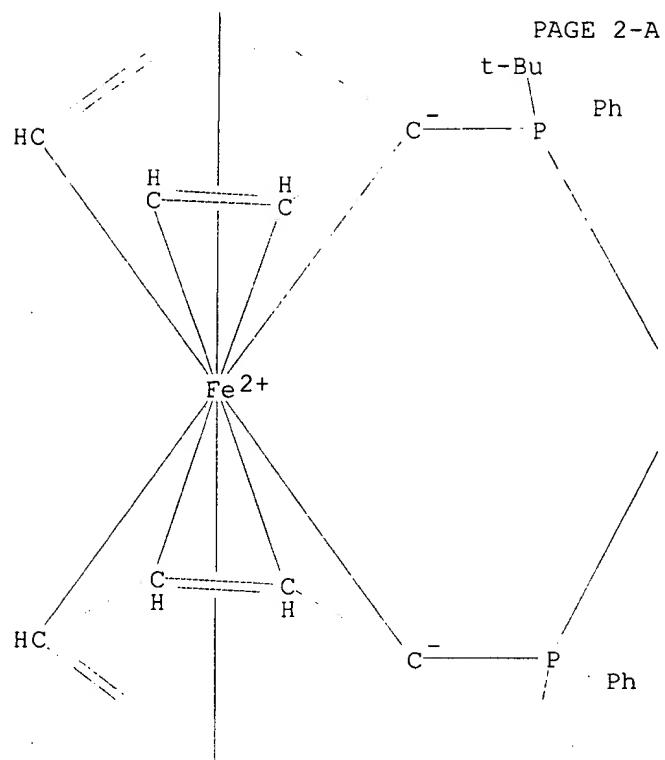
RN 92269-95-9 HCAPLUS

CN Rhodium(1+), [(2,3,5,6- η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis[(1,1'-dimethylethyl)phenylphosphino]ferrocene-P,P']-, stereoisomer, perchlorate
(9CI) (CA INDEX NAME)

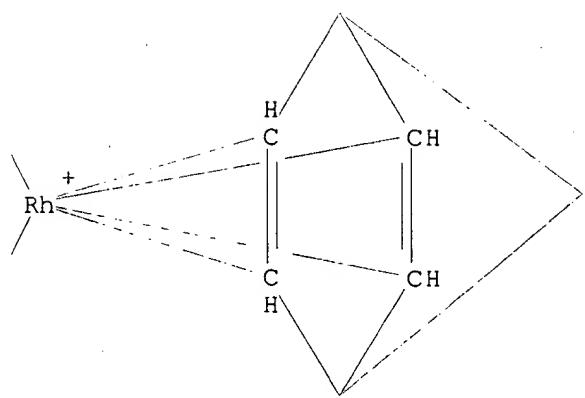
CM 1

CRN 92269-94-8
CMF C37 H44 Fe P2 Rh
CCI CCS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

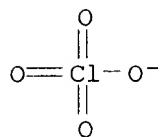


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PAGE 3-A
t-Bu

CM 2

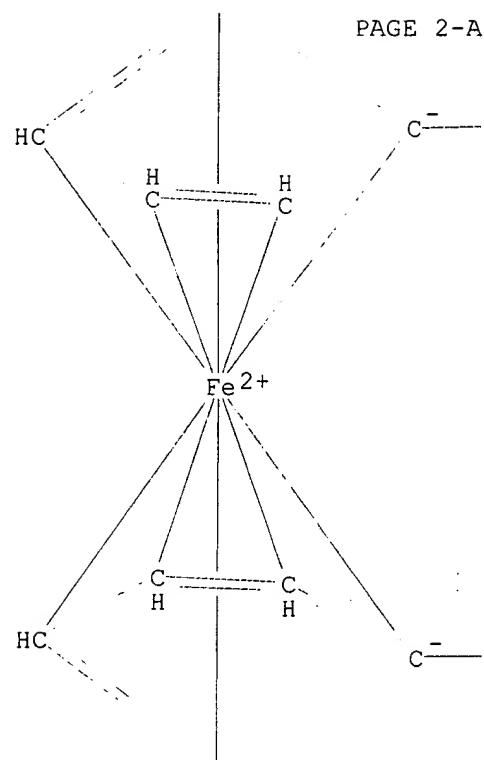
CRN 14797-73-0
CMF Cl O4RN 92284-07-6 HCPLUS
CN Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1-[bis(1,1-dimethylethyl)phosphino]-1'-(diphenylphosphino)ferrocene-P,P']-, perchlorate (9CI) (CA INDEX NAME)

CM 1

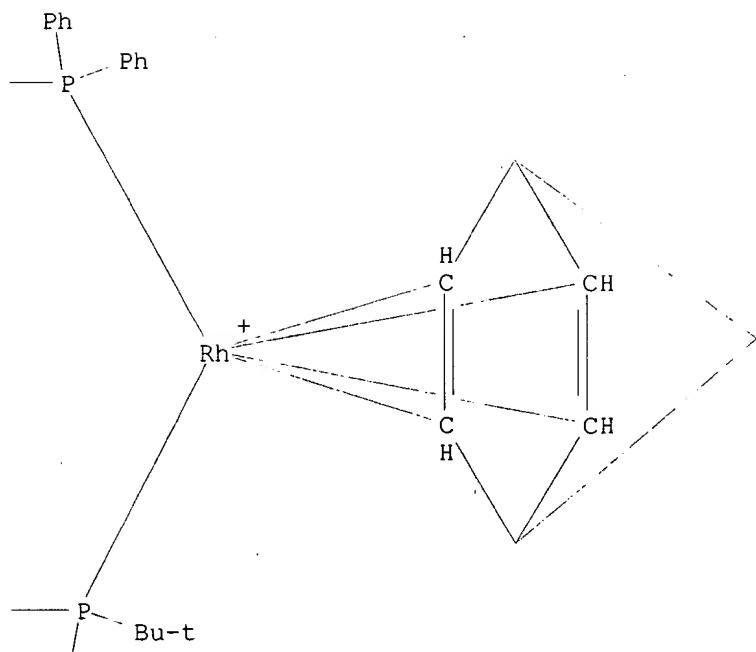
CRN 92284-06-5
CMF C37 H44 Fe P2 Rh
CCI CCS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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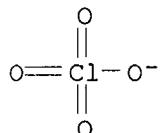
PAGE 3-A

C
H

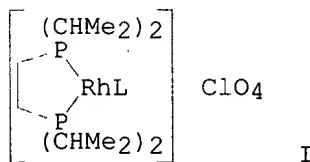
PAGE 3-B

t-Bu

CM 2

CRN 14797-73-0
CMF Cl O4

L104 ANSWER 14 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN
 AN 1985:185249 HCAPLUS
 DN 102:185249
 ED Entered STN: 02 Jun 1985
 TI **Hydrogenation** of cationic bis(tertiary alkylphosphine)
rhodium(I) complexes. An NMR study
 AU Butler, Ian R.; Cullen, William R.; Mann, Brian E.; Nurse, Charles R.
 CS Dep. Chem., Univ. British Columbia, Vancouver, BC, V6T 1Y6, Can.
 SO Journal of Organometallic Chemistry (1985), 280(2), C47-C50
 CODEN: JORCAI; ISSN: 0022-328X
 DT Journal
 LA English
 CC 29-13 (Organometallic and Organometalloidal Compounds)
 GI



AB Rhodium hydrides have been observed in solution in the reaction of cationic **rhodium(I)** complexes of bis(tertiary phosphines), e.g., (I, L = norbornadiene) with H.
 ST **hydrogenation phosphinerhodium complex;**

rhodium phosphine hydrogenation; hydride rhodium phosphine; NMR hydrogenation phosphinerhodium complex
IT Nuclear magnetic resonance
(of hydrogenation of rhodium phosphine complexes)

Hydrogenation
(of rhodium phosphine complexes)

IT 84680-96-6 92269-95-9 96144-39-7 96144-63-7
96144-65-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrogenation of)
IT 96144-41-1P 96144-67-1P 96144-69-3P
96144-71-7P 96144-73-9P 96144-75-1P
96144-77-3DP, perchlorate derivative
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT 84680-96-6 92269-95-9 96144-63-7
96144-65-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrogenation of)

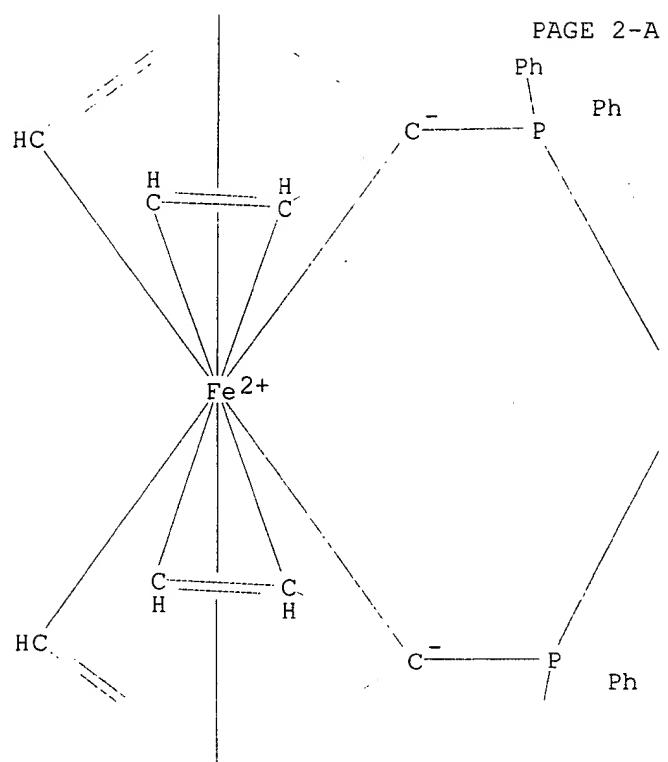
RN 84680-96-6 HCAPLUS

CN Rhodium(1+), [(2,3,5,6- η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis(diphenylphosphino- κ P)ferrocene]-, perchlorate (9CI) (CA INDEX NAME)

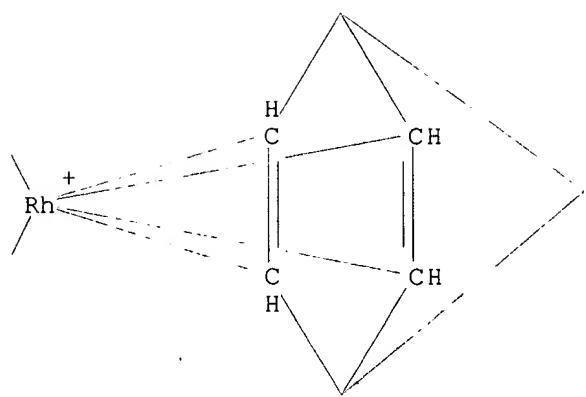
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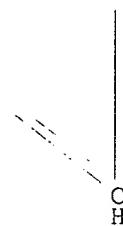
CRN 79790-97-9
CMF C41 H36 Fe P2 Rh
CCI CCS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *



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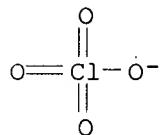




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Ph

CM 2

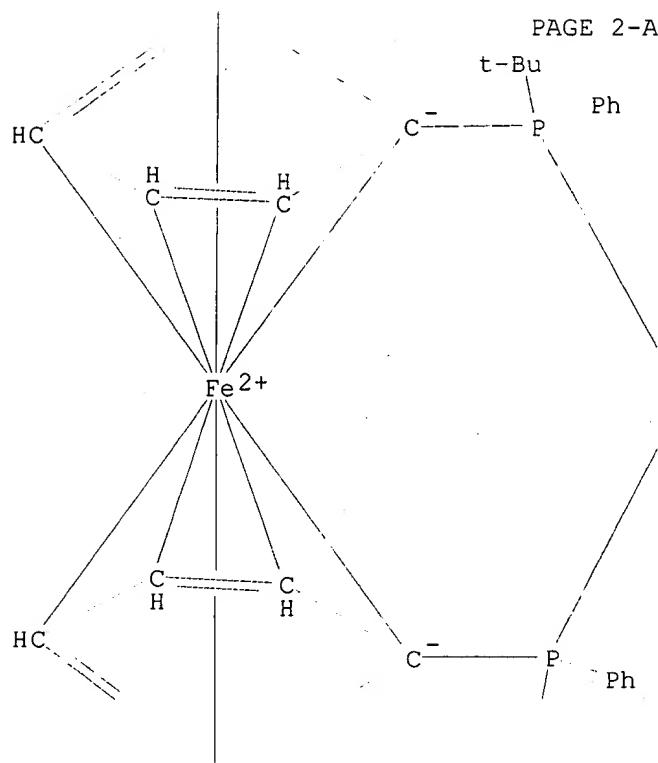
CRN 14797-73-0
CMF Cl O4RN 92269-95-9 HCAPLUS
CN Rhodium(1+), [(2,3,5,6- η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis[(1,1-dimethylethyl)phenylphosphino]ferrocene-P,P']-, stereoisomer, perchlorate (9CI) (CA INDEX NAME)

CM 1

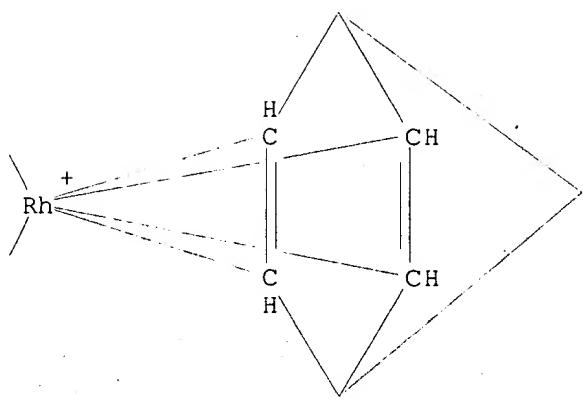
CRN 92269-94-8
CMF C37 H44 Fe P2 Rh
CCI CCS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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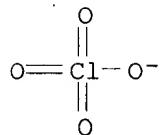


PAGE 3-A
t-Bu

C
H

CM 2

CRN 14797-73-0
CMF C1 O4



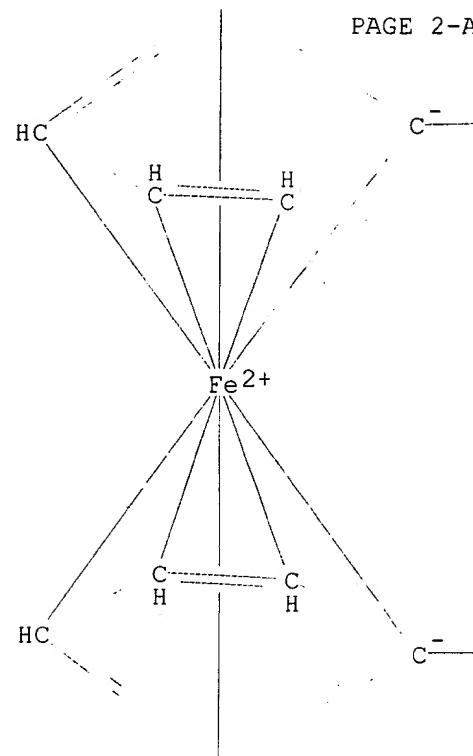
RN 96144-63-7 HCAPLUS
CN Rhodium(1+), [(2,3,5,6- η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis[bis(1-methylethyl)phosphino]ferrocene-P,P']-, perchlorate (9CI) (CA INDEX NAME)

CM 1

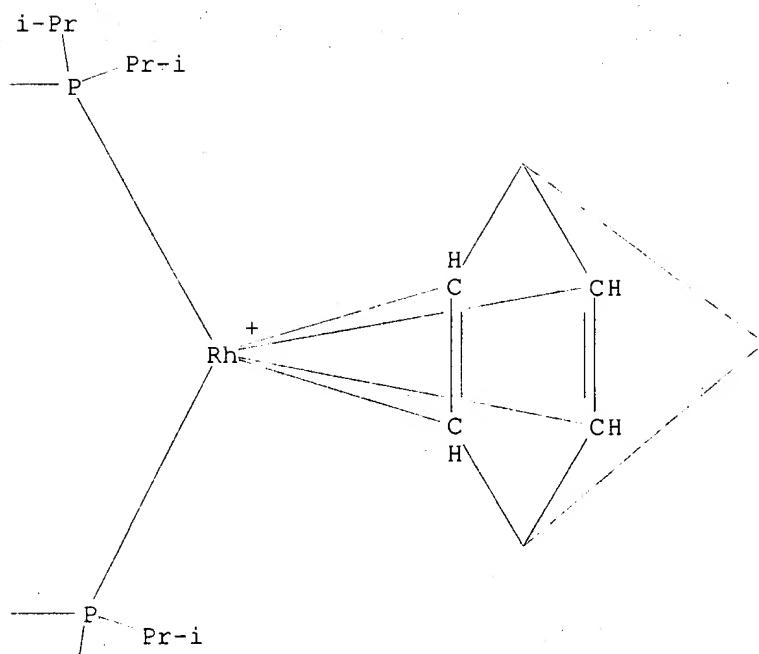
CRN 96144-62-6
CMF C29 H44 Fe P2 Rh
CCI CCS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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PAGE 3-A

C
H

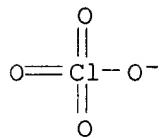
PAGE 3-B

i-Pr

CM 2

CRN 14797-73-0

CMF Cl O4



RN 96144-65-9 HCPLUS

CN Rhodium(1+), [(2,3,5,6- η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis[(1-methylethyl)phenylphosphino]ferrocene-P,P']-, perchlorate (9CI) (CA INDEX NAME)

CM 1

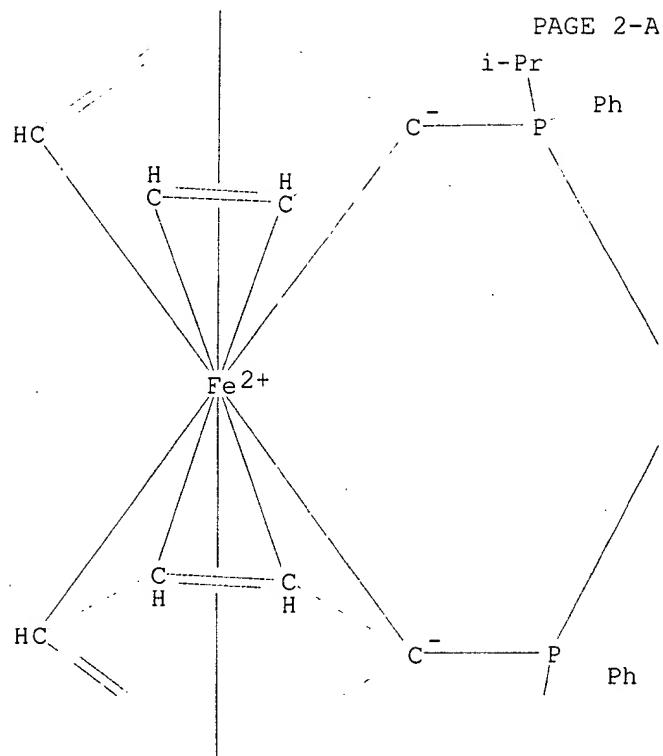
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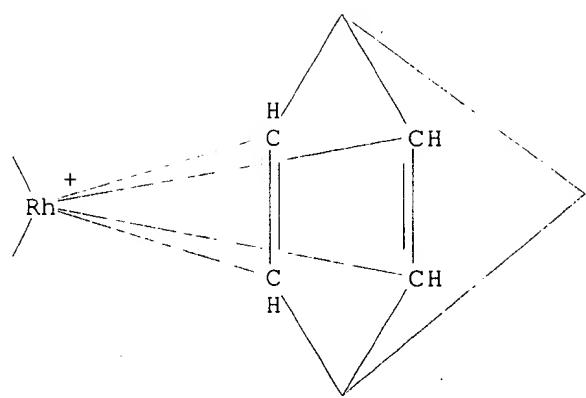
CCI CCS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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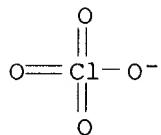
PAGE 2-B



PAGE 3-A
i-Pr

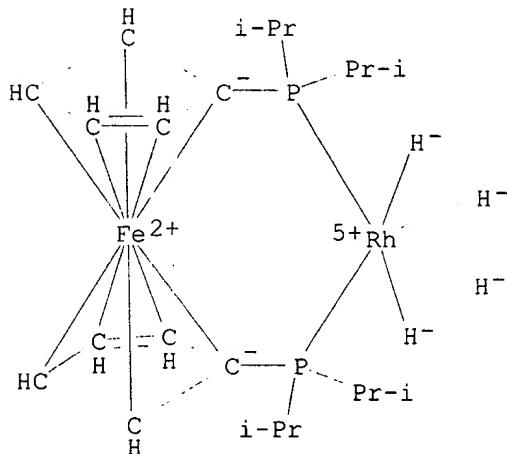


CM 2

CRN 14797-73-0
CMF Cl O4

IT 96144-67-1P 96144-69-3P 96144-71-7P
 96144-73-9P 96144-75-1P 96144-77-3DP,
 perchlorate derivative
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 96144-67-1 HCAPLUS
 CN Rhodium(1+), [1,1'-bis[bis(1-methylethyl)phosphino]ferrocene-
 P,P']tetrahydro-, perchlorate (9CI) (CA INDEX NAME)

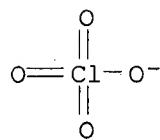
CM 1

CRN 96144-66-0
CMF C22 H40 Fe P2 Rh
CCI CCS

CM 2

CRN 14797-73-0

CMF Cl O4



RN 96144-69-3 HCPLUS

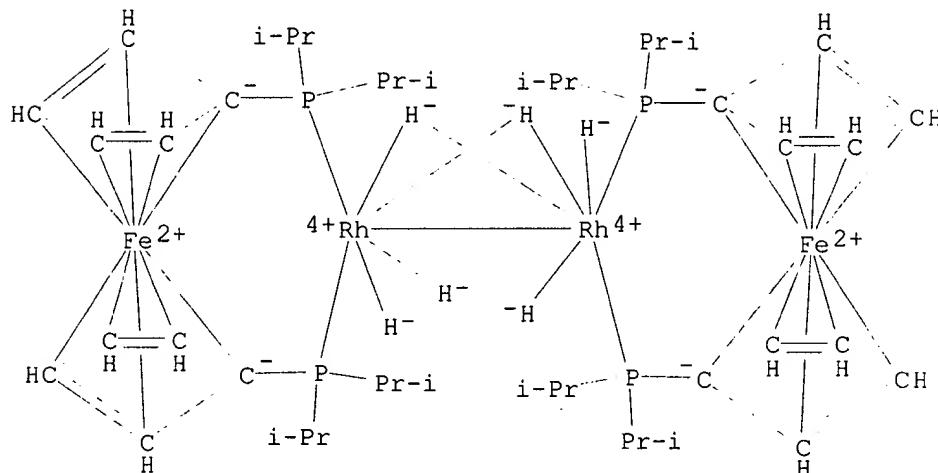
CN Rhodium(2+), bis[1,1'-bis[bis(1-methylethyl)phosphino]ferrocene-P,P']di- μ -hydrotetrahydrodi-, (Rh-Rh), diperchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 96144-68-2

CMF C44 H78 Fe2 P4 Rh2

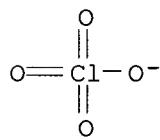
CCI CCS



CM 2

CRN 14797-73-0

CMF Cl O4



RN 96144-71-7 HCPLUS

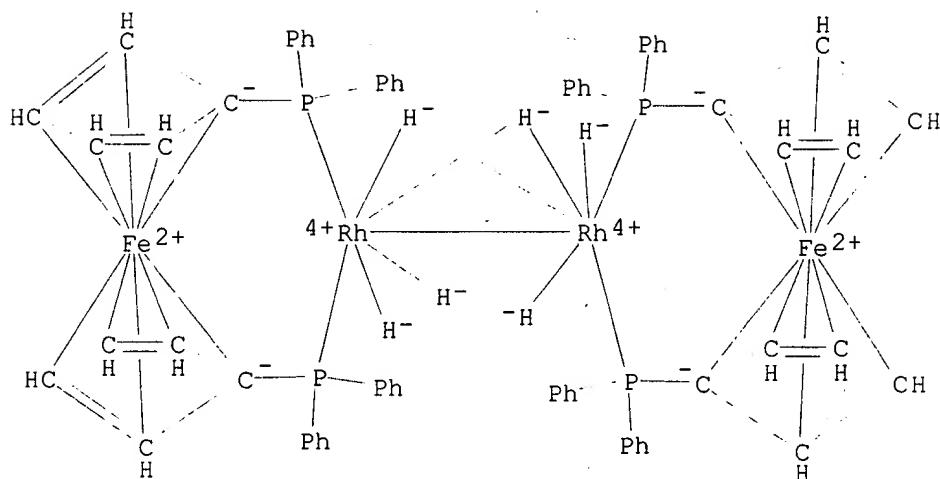
CN Rhodium(2+), bis[1,1'-bis(diphenylphosphino)ferrocene-P,P']di- μ -hydrotetrahydrodi-, (Rh-Rh), diperchlorate (9CI) (CA INDEX NAME)

CM 1

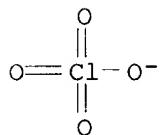
CRN 96144-70-6

CMF C68 H62 Fe2 P4 Rh2

CCI CCS



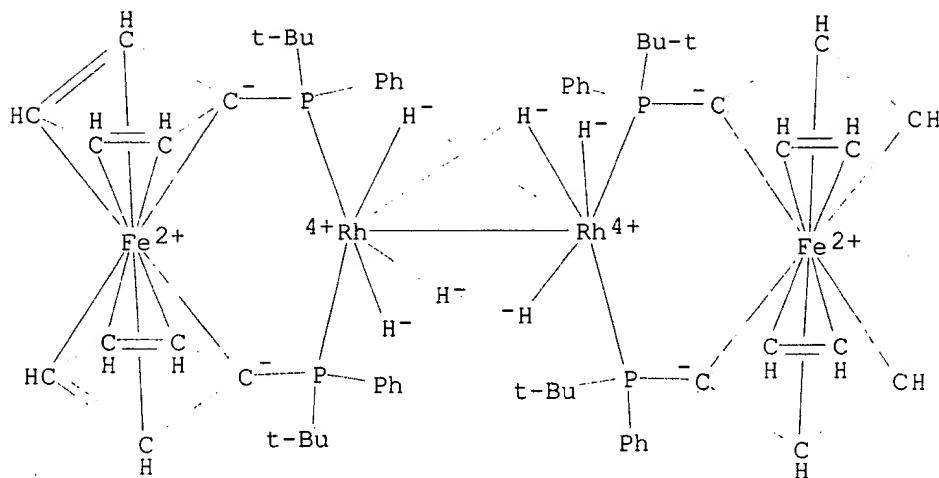
CM 2

CRN 14797-73-0
CMF Cl O4

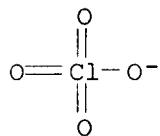
RN 96144-73-9 HCPLUS
 CN Rhodium(2+), bis[1,1'-bis[(1,1-dimethylethyl)phenylphosphino]ferrocene-P,P']di- μ -hydrotetrahydrodi-, (Rh-Rh), diperchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 96144-72-8
CMF C60 H78 Fe2 P4 Rh2
CCI CCS

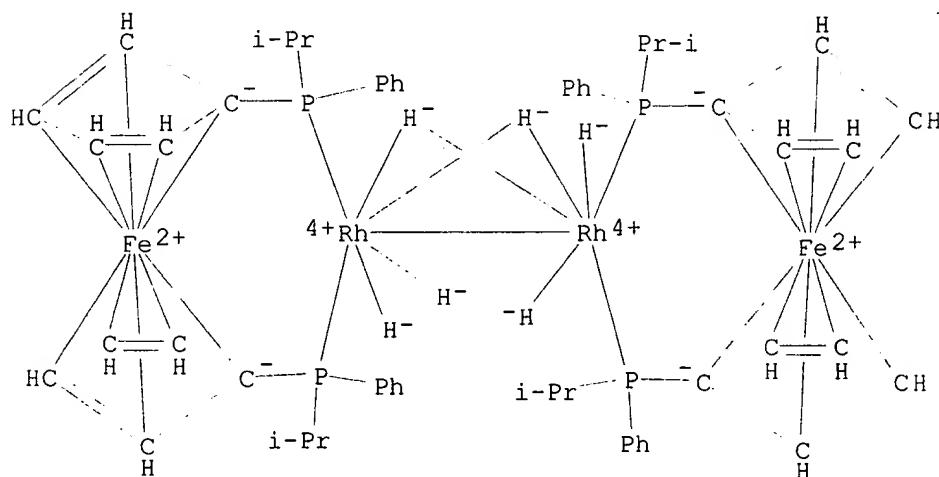


CM 2

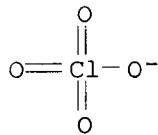
CRN 14797-73-0
CMF C1 O4

RN 96144-75-1 HCAPLUS
 CN Rhodium(2+), bis[1,1'-bis[(1-methylethyl)phenylphosphino]ferrocene-P,P']di-
 μ-hydrotetrahydrodi-, (Rh-Rh), diperchlorate (9CI) (CA INDEX NAME)

CM 1

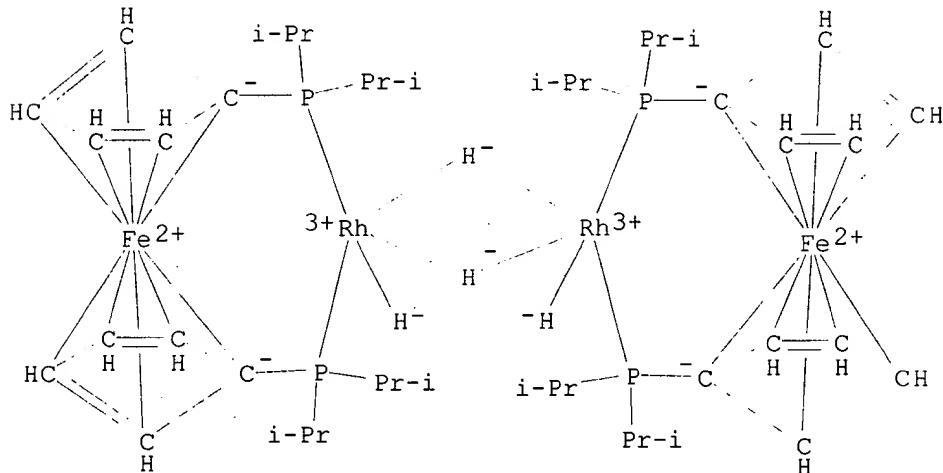
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 CMF C56 H70 Fe2 P4 Rh2
 CCI CCS

CM 2

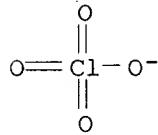
CRN 14797-73-0
CMF Cl O4

RN 96144-77-3 HCAPLUS
 CN Rhodium(2+), bis[1,1'-bis[bis(1-methylethyl)phosphino]ferrocene-P, P']di-
 μ-hydrodihydrodi-, diperchlorate (9CI) (CA INDEX NAME)

CM 1

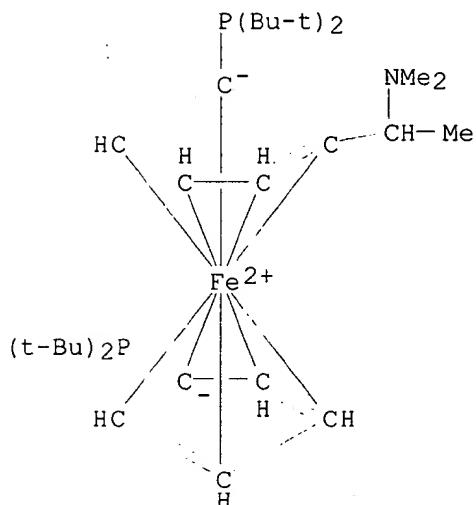
CRN 96144-76-2
CMF C44 H76 Fe2 P4 Rh2
CCI CCS

CM 2

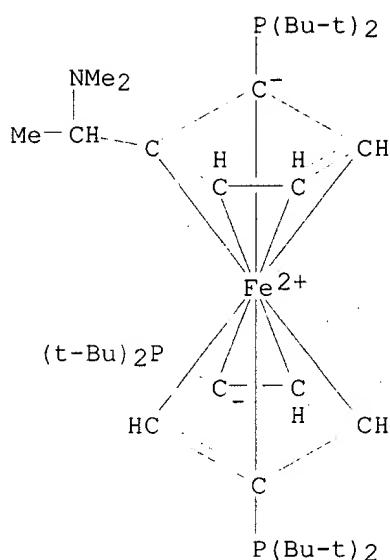
CRN 14797-73-0
CMF Cl O4

ED Entered STN: 18 May 1985
 TI Rhodium(I) complexes of ferrocenylphosphines as efficient asymmetric catalysts. The structure of $\text{Fe}(\eta^5\text{-C}_5\text{H}_3(\text{P}(\text{CMe}_3)_2-1,3)(\eta^5\text{-C}_5\text{H}_3(\text{CHMeNMe}_2)\text{P}(\text{CMe}_3)_2-1,2)$
 AU Appleton, Trevor D.; Cullen, William R.; Evans, Stephen V.; Kim, Tae Jeong; Trotter, James
 CS Dep. Chem., Univ. Br. Columbia, Vancouver, BC, V6T 1Y6, Can.
 SO Journal of Organometallic Chemistry (1985), 279(1-2), 5-21
 CODEN: JORCAI; ISSN: 0022-328X
 DT Journal
 LA English
 CC 29-13 (Organometallic and Organometalloidal Compounds)
 Section cross-reference(s): 23, 25, 67, 75
 OS CASREACT 102:166925
 GI For diagram(s), see printed CA Issue.
 AB The chiral aminomethylferrocenes (R)- or (S)-I ($\text{R}-\text{R}_2 = \text{H}$) were lithiated and treated with $\text{ClP}(\text{CMe}_3)_2$ under varying reaction conditions to give (R,S)-I [$\text{R} = \text{P}(\text{CMe}_3)_2$; $\text{R}_1 = \text{H}$ (II), $\text{P}(\text{CMe}_3)_2$ (III); $\text{R}_2 = \text{H}$] and (S,R)-I (same R's) resp. Similarly, (R, R)- or (S, S)-I [$\text{R} = \text{R}_2 = \text{P}(\text{CMe}_3)_2$, $\text{R}_1 = \text{H}$] (IV) were prepared from (R)- or (S)-I ($\text{R}-\text{R}_2 = \text{H}$) resp. [Rh (NBD)L]ClO₄ [V; NBD = norbornadiene, L = (S,R)-II, (S,R-III, (S,S)-IV) catalyzed asym **hydrogenation** of $\text{H}_2\text{C:CR}_3\text{CO}_2\text{H}$ ($\text{R}_3 = \text{Me, CH}_2\text{CO}_2\text{H}$) and $\text{PhCH:CR}_4\text{CO}_2\text{H}$ ($\text{R}_4 = \text{NHAc, Me}$); V [L = (S,S)-IV] gave products with up to 95% enantiomeric excesses. The x-ray crystal structure of (S,S)-IV showed the cyclopentadienyl rings are close to planar, deviate slightly from coplanarity, and are rotated by about 7° from an eclipsed conformation. The substituent P and C atoms are significantly displaced from the ring planes.
 ST crystal structure ferrocenyltriphosphine chiral; mol structure ferrocenyltriphosphine chiral; ferrocenylphosphine structure **rhodium** complex catalyst; **rhodium** ferrocenylphosphine complex **hydrogenation** asym
 IT Crystal structure
 Molecular structure
 (of ferrocenyltriphosphine complex, chiral)
 IT Asymmetric synthesis and induction
 (of organic acids, by **hydrogenation** of olefinic acids, **rhodium**-ferrocenylphosphine catalyst for)
 IT **Hydrogenation**
 (asym., of olefinic acids)
 IT **Hydrogenation catalysts**
 (asym., **rhodium**-ferrocenyltriphosphine complex, for olefinic acids)
 IT 97-65-4, reactions 1895-97-2 5429-56-1 55065-02-6
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (asym. **hydrogenation** of, **rhodium**-ferrocenylphosphine complex for)
 IT 95840-92-9
 RL: CAT (Catalyst use); USES (Uses)
 (catalyst, for asym. **hydrogenation** of olefinic acids)
 IT 83356-93-8 95839-80-8
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (complexation of, with **rhodium** complex)
 IT 31886-57-4 31886-58-5
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (lithiation and phosphination of)
 IT 95762-74-6P 95839-79-5P 95840-91-8P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and complexation of, with **rhodium**)
 IT 95839-76-2P 95839-78-4P 95840-90-7P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (preparation and conformation of)
 IT 97-69-8P 2018-61-3P 2174-58-5P 3641-51-8P 10172-89-1P

14367-54-5P 14367-67-0P 19436-52-3P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, by asym. **hydrogenation** of olefinic acid,
 rhodium-ferrocenyltriphosphine complex for)
 IT 95762-71-3P 95762-73-5P 95840-45-2P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation, conformation, and catalyst activity of, for asym.
hydrogenation)
 IT 95762-75-7P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation, crystal structure, and complexation of, with **rhodium**)
)
 IT 13716-10-4
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with chiral aminoferrocene)
 IT 95762-74-6P 95839-79-5P 95840-91-8P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and complexation of, with **rhodium**)
 RN 95762-74-6 HCPLUS
 CN Ferrocene, 1,1'-bis[bis(1,1-dimethylethyl)phosphino]-2-[1-(dimethylamino)ethyl]-, [R-(R*,R*)]- (9CI) (CA INDEX NAME)

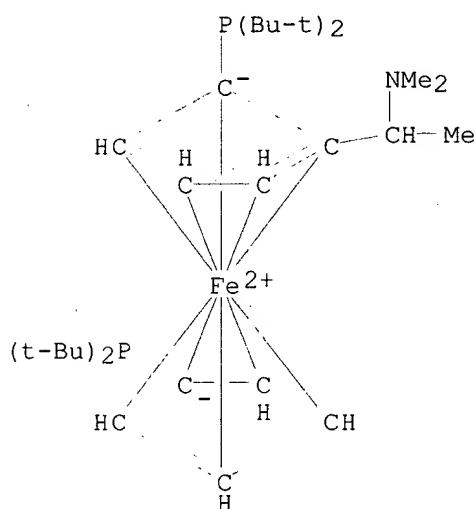


RN 95839-79-5 HCPLUS
 CN Ferrocene, 1,1',3'-tris[bis(1,1-dimethylethyl)phosphino]-2-[1-(dimethylamino)ethyl]-, [S-(R*,S*)]- (9CI) (CA INDEX NAME)



RN 95840-91-8 HCPLUS

CN Ferrocene, 1,1'-bis[bis(1,1-dimethylethyl)phosphino]-2-[1-(dimethylamino)ethyl]-, [S-(R*,R*)]- (9CI) (CA INDEX NAME)



IT 95839-76-2P 95839-78-4P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and conformation of)

RN 95839-76-2 HCPLUS

CN Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis[bis(1,1-dimethylethyl)phosphino]-2-[1-(dimethylamino)ethyl]ferrocene-N2,P1]-, [R-(R*,R*)]-, perchlorate (9CI) (CA INDEX NAME)

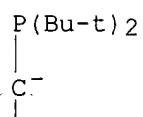
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CRN 95839-75-1

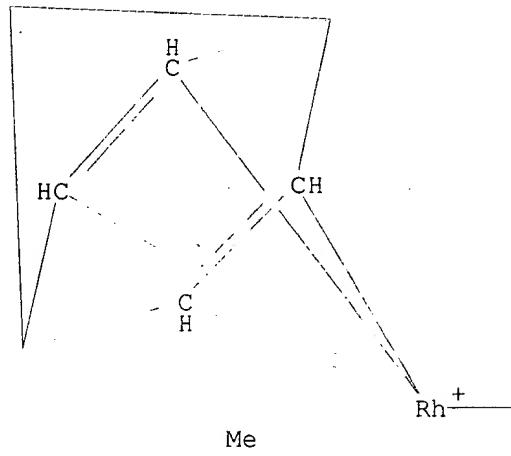
CMF C37 H61 Fe N P2 Rh

CCI CCS

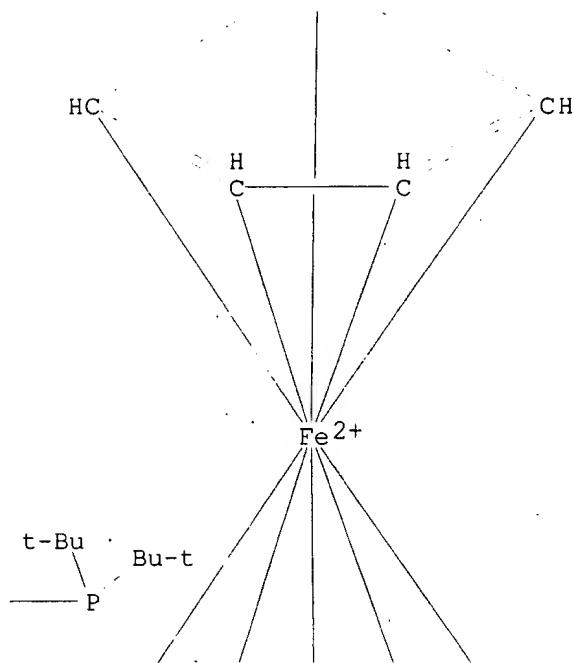
PAGE 1-B



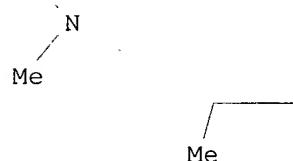
PAGE 2-A



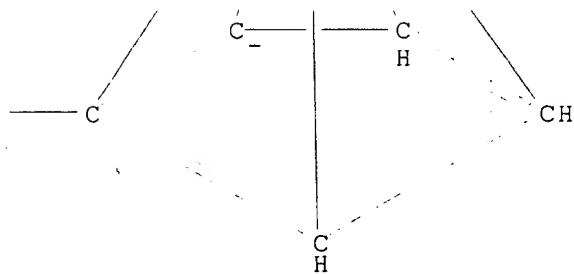
PAGE 2-B



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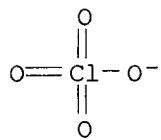


PAGE 3-B



CM 2

CRN 14797-73-0
CMF Cl O4



RN 95839-78-4 HCPLUS

CN Rhodium(1+), [(2,3,5,6- η)-bicyclo[2.2.1]hepta-2,5-diene][1,1',3'-tris[bis(1,1-dimethylethyl)phosphino]-2-[1-(dimethylamino)ethyl]ferrocene-N2,P1]-, [S-(R*,S*)]-, perchlorate (9CI) (CA INDEX NAME)

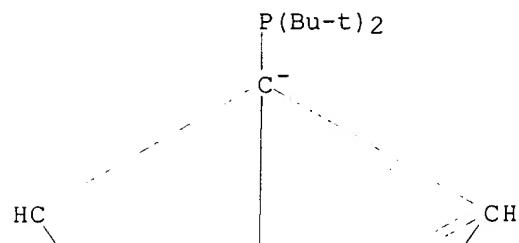
CM 1

CRN 95839-77-3

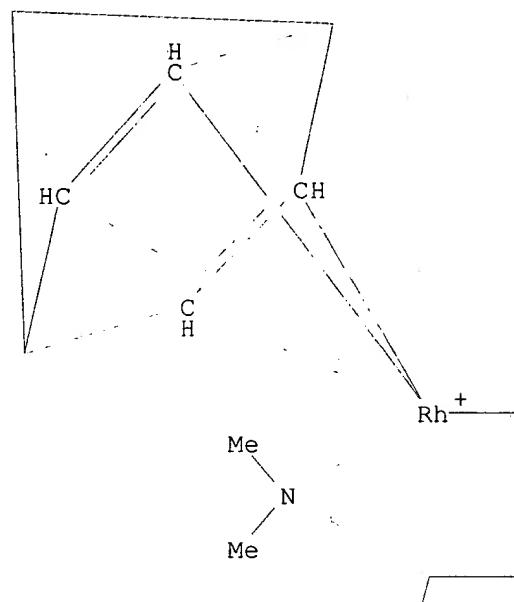
CMF C45 H78 Fe N P3 Rh

CCI CCS

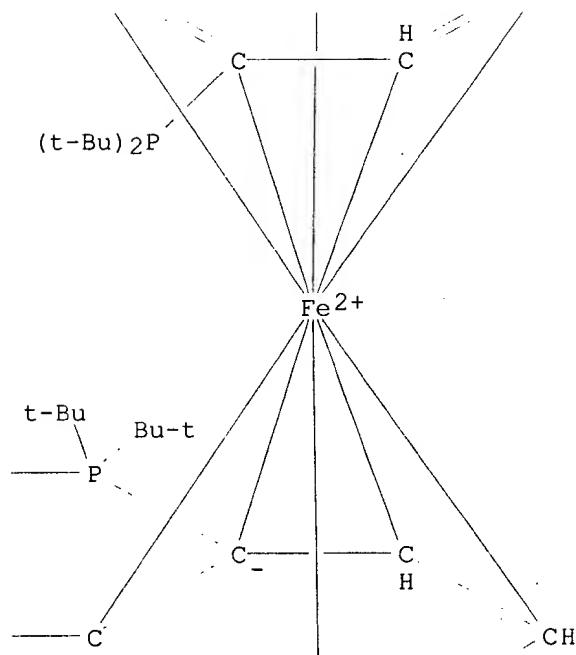
PAGE 1-B



PAGE 2-A



PAGE 2-B



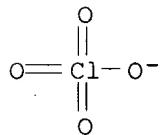
PAGE 3-A

Me

PAGE 3-B



CM 2

CRN 14797-73-0
CMF Cl O4

IT 95762-71-3P 95762-73-5P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, conformation, and catalyst activity of, for asym.
hydrogenation)

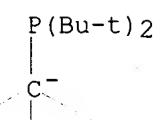
RN 95762-71-3 HCAPLUS

CN Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-
bis[bis(1,1-dimethylethyl)phosphino]-2-[1-(dimethylamino)ethyl]ferrocene-
N2,P1]-, stereoisomer, perchlorate (9CI) (CA INDEX NAME)

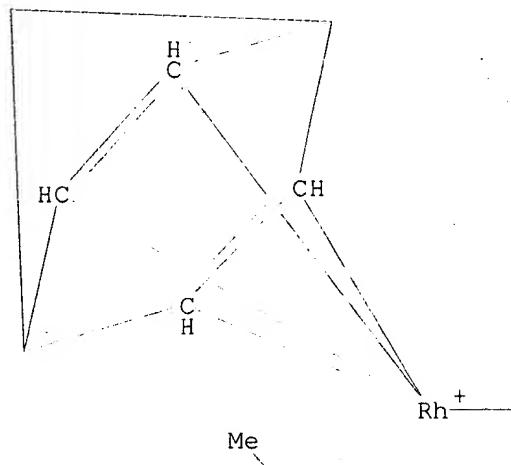
CM 1

CRN 95762-70-2
CMF C37 H61 Fe N P2 Rh
CCI CCS

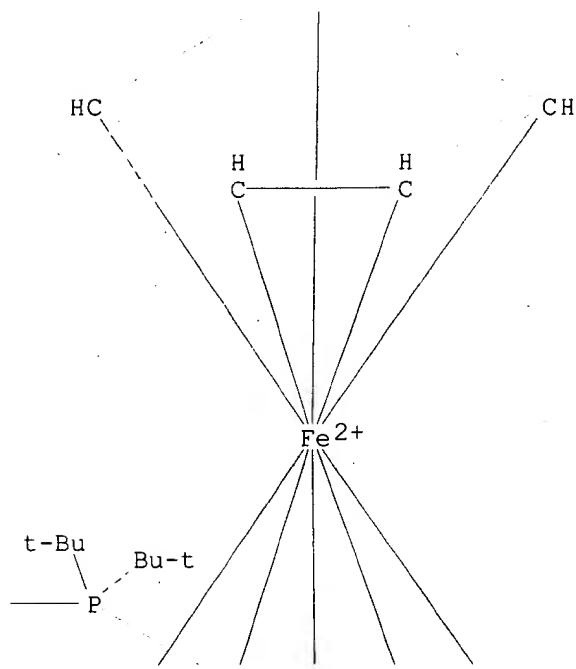
PAGE 1-B



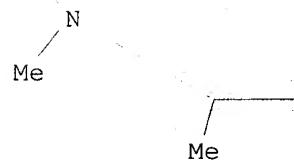
PAGE 2-A



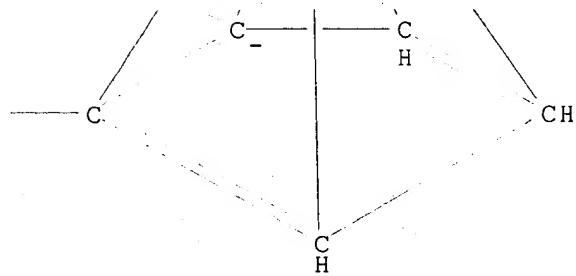
PAGE 2-B



PAGE 3-A

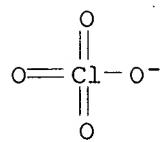


PAGE 3-B



CM 2

CRN 14797-73-0
CMF Cl 04



RN 95762-73-5 HCPLUS

CN Rhodium(1+), [(2,3,5,6- η)-bicyclo[2.2.1]hepta-2,5-diene][1,1',3-tris[bis(1,1-dimethylethyl)phosphino]-2'-(1-(dimethylamino)ethyl)ferrocene-N2',P1']-, stereoisomer, perchlorate (9CI) (CA INDEX NAME)

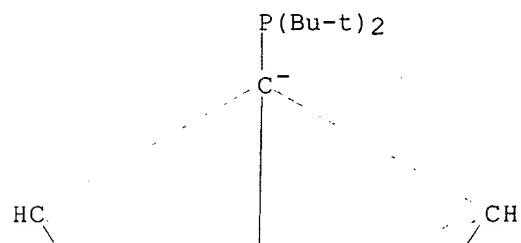
CM 1

CRN 95762-72-4

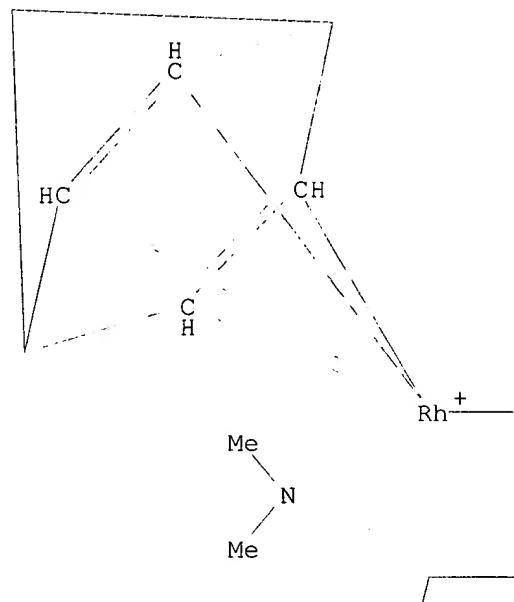
CMF C45 H78 Fe N P3 Rh

CCI CCS

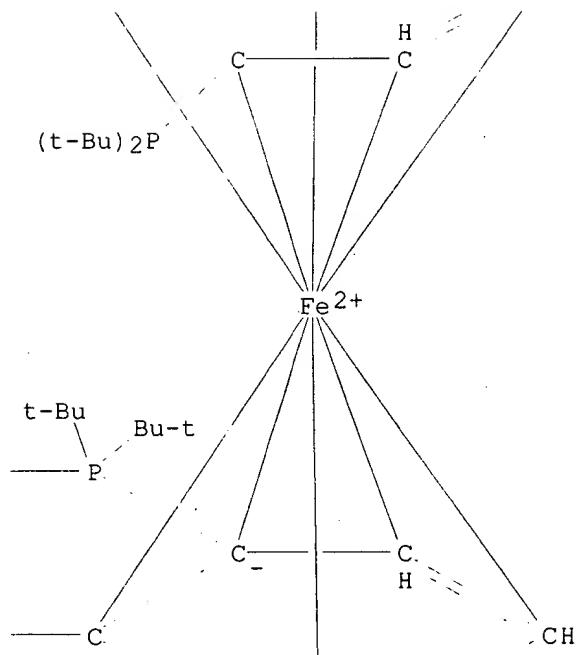
PAGE 1-B



PAGE 2-A



PAGE 2-B



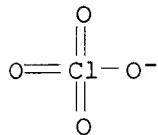
PAGE 3-A

Me

PAGE 3-B



CM 2

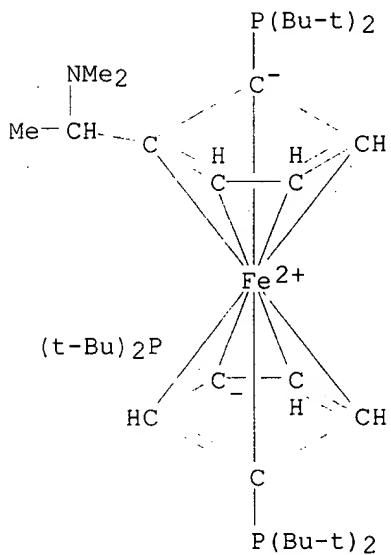
CRN 14797-73-0
CMF Cl 04

IT 95762-75-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, crystal structure, and complexation of, with rhodium
)

RN 95762-75-7 HCAPLUS

CN Ferrocene, 1,1',3'-tris[bis(1,1-dimethylethyl)phosphino]-2-[1-(dimethylamino)ethyl]-, [R-(R*,S*)]- (9CI) (CA INDEX NAME)



L104 ANSWER 16 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1985:158448 HCAPLUS

DN 102:158448

ED Entered STN: 04 May 1985

TI Crystallographic analysis of two rhodium(III) hydride complexes,
bis[1,1'-bis[tert-butyl(phenyl)phosphino]ferrocene-P,P']-tri- μ -hydrido-

dihydridodirhodium(III) chlorate methanol solvate, [Rh₂H₅{Fe[P(C₄H₉)(C₅H₄)(C₆H₅)]₂}₂]ClO₄.CH₃OH (I), and bis[1,1'-bis(di-tert-butylphosphino)ferrocene-P,P']-tri- μ -hydrido-dihydridodirhodium(III) chlorate, [Rh₂H₅{Fe[P(C₄H₉)₂(C₅H₄)]₂}₂]ClO₄ (II)

AU Einstein, F. W. B.; Jones, T.

CS Dep. Chem., Simon Fraser Univ., Burnaby, BC, V5A 1S6, Can.

SO Acta Crystallographica, Section C: Crystal Structure Communications (1985), C41(3), 365-9

CODEN: ACSCEE; ISSN: 0108-2701

DT Journal

LA English

CC 75-8 (Crystallography and Liquid Crystals)
Section cross-reference(s): 29, 78

AB Title compound (I) is monoclinic, space group P21/n, with a 18.708(4), b 14.857(2), c 21.853(4) Å, and β 92.95(2) $^\circ$; Z = 4 for d = 1.501. The final R = 0.045 for 5732 reflections. Title compound (II) is monoclinic, space group P21/c, with a 15.276(3), b 14.751(2), c 25.950(3) Å, and β 90.85(1) $^\circ$; Z = 4, for d = 1.430. The final R = 0.059 for 4180 reflections. The structure of I contains an unusual RhPH skeletal structure in which each Rh atom (in the 3+ oxidation state) has 3 Rh-H bridging bonds [average 1.77(8) Å], a single Rh-H terminal bond [average 1.56(12) Å] and 2 Rh-P bonds. It is tentatively proposed that II contains a similar arrangement. Atomic coordinates are given.

ST mol structure rhodium hydro bridged phosphinoferrocene; ferrocene butylphosphino rhodium hydro structure

IT Crystal structure
Molecular structure
(of rhodium hydro-bridged butylphenylphosphinoferrocene and dibutylphosphinoferrocene complexes)

IT 92468-68-3 95783-24-7
RL: PRP (Properties)
(structure of)

IT 92468-68-3
RL: PRP (Properties)
(structure of)

RN 92468-68-3 HCAPLUS

CN Rhodium(1+), bis[1,1'-bis[(1,1-dimethylethyl)phenylphosphino]ferrocene-P,P']tri- μ -hydrido-*di*hydro-, stereoisomer, perchlorate, compd. with methanol (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 67-56-1
CMF C H₄ O

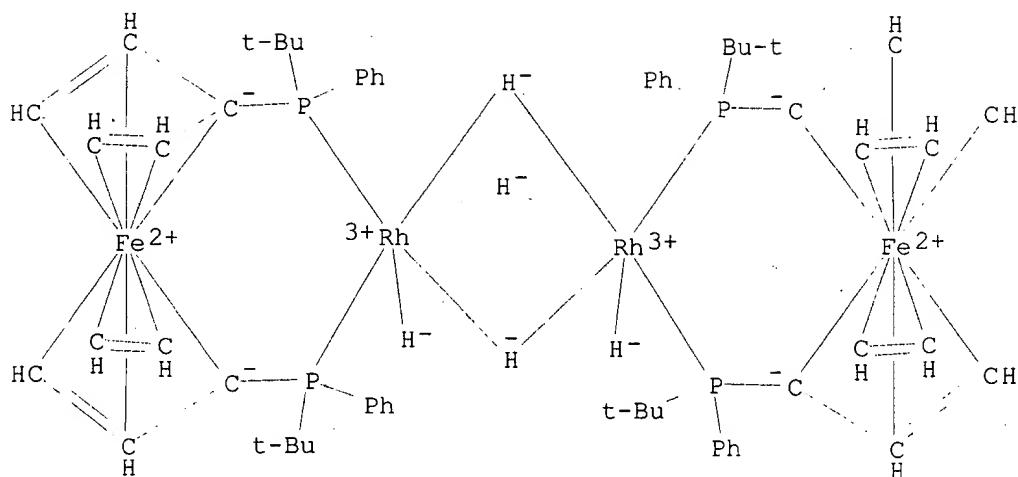
H₃C-OH

CM 2

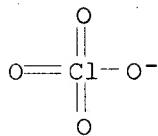
CRN 92468-67-2
CMF C₆O H₇ Fe₂ P₄ Rh₂ . Cl O₄

CM 3

CRN 92468-66-1
CMF C₆O H₇ Fe₂ P₄ Rh₂
CCI CCS



CM 4

CRN 14797-73-0
CMF Cl O4

L104 ANSWER 17 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1985:79103 HCAPLUS

DN 102:79103

ED Entered STN: 09 Mar 1985

TI Structures of three **hydrogenation** catalysts $[(\text{P-P})\text{Rh}(\text{NBD})]\text{ClO}_4$ and some comparative rate studies where $(\text{P-P}) = (\eta^5\text{-R}_1\text{R}_2\text{P}\text{C}_5\text{H}_4)(\eta^5\text{-R}_3\text{R}_4\text{P}\text{C}_5\text{H}_4)\text{Fe}$ ($\text{R}_1 = \text{R}_2 = \text{R}_3 = \text{R}_4 = \text{Ph}$; $\text{R}_1 = \text{R}_2 = \text{Ph}$, $\text{R}_3 = \text{R}_4 = \text{CMe}_3$; $\text{R}_1 = \text{R}_3 = \text{Ph}$, $\text{R}_2 = \text{R}_4 = \text{CMe}_3$)

AU Cullen, William R.; Kim, Tae Jeong; Einstein, Frederick W. B.; Jones, Terry

CS Chem. Dep., Univ. British Columbia, Vancouver, BC, V6T 1Y6, Can.

SO Organometallics (1985), 4(2), 346-51

CODEN: ORGND7; ISSN: 0276-7333

DT Journal

LA English

CC 29-13 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 22

AB Bulky Me_3C groups enhance the **hydrogenation** rates of alkenes (except for bulky substrates) at $30^\circ/1$ atm H_2 using the title compds. $[(\text{P-P})\text{RhNBD}]\text{ClO}_4$ $[(\text{P-P}) = (\eta^5\text{-R}_1\text{R}_2\text{P}\text{C}_5\text{H}_4)\text{Fe}(\eta^5\text{-R}_3\text{R}_4\text{P}\text{C}_5\text{H}_4)]$; $\text{R}_1 = \text{R}_2 = \text{R}_3 = \text{R}_4 = \text{Me}_3\text{C}$ (I), Ph (II); $\text{R}_1 = \text{R}_2 = \text{Me}_3\text{C}$, $\text{R}_3 = \text{R}_4 = \text{Ph}$ (III); $\text{R}_1 = \text{R}_3 = \text{Me}_3\text{C}$, $\text{R}_2 = \text{R}_4 = \text{Ph}$ (IV) as catalyst precursors. The most promising combination of steric and electronic effects exists with (±)-IV. Crystallog. of II, III, and IV show that the bulky Me_3C groups cause a lengthening of P-Rh distances, wider P-Rh-P angles, and a rotation of the norbornadiene group out of the P-Rh-P plane. Generally the effects range from a maximum in I (previously determined)

to a min. in III.

ST crystal structure **rhodium** phosphine complex; mol structure
rhodium phosphine complex; steric effect **hydrogenation**
catalyst; ferrocenebisphosphine **rhodium** complex butyl group

IT tert-Butyl group
(effect of, on **hydrogenation** of alkenes using
ferrocenebis(phosphine)**rhodium** complex catalyst)

IT **Hydrogenation catalysts**
(ferrocenebis(phosphine) **rhodium** complexes, for alkenes,
kinetics and mechanism with)

IT Alkenes, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(**hydrogenation** of, **rhodium** phosphine catalyst for)

IT Bond angle
Bond length
(in ferrocenebis(phosphine) **rhodium** complexes)

IT Kinetics of **hydrogenation**
(of alkenes in presence of ferrocenebis(phosphine) **rhodium**
complexes)

IT **Hydrogenation**
(of alkenes in presence of ferrocenebis(phosphine) **rhodium**
complexes, mechanism of)

IT Crystal structure
Molecular structure
(of ferrocenebis(phosphine) **rhodium** complexes)

IT Substituent effect
(on catalytic activity of ferrocene bis(phosphine)**rhodium**
complex in **hydrogenation** of alkenes)

IT Steric effect
(on **hydrogenation** of alkenes using ferrocenebis(phosphine)
rhodium complexes)

IT 84680-96-6 92269-95-9 92284-07-6
RL: CAT (Catalyst use); USES (Uses)
(catalyst, for **hydrogenation** of alkenes, crystallog. in
relation to kinetics and mechanism with)

IT 84680-98-8
RL: CAT (Catalyst use); USES (Uses)
(catalyst, for **hydrogenation** of alkenes, mol. structure in
relation to kinetics and mechanism with)

IT 97-65-4, reactions 110-83-8, reactions 1199-77-5 5429-56-1
5469-45-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(**hydrogenation** of, using ferrocenebis(phosphine)
rhodium complexes, kinetics and mechanism of)

IT 84680-96-6 92269-95-9 92284-07-6
RL: CAT (Catalyst use); USES (Uses)
(catalyst, for **hydrogenation** of alkenes, crystallog. in
relation to kinetics and mechanism with)

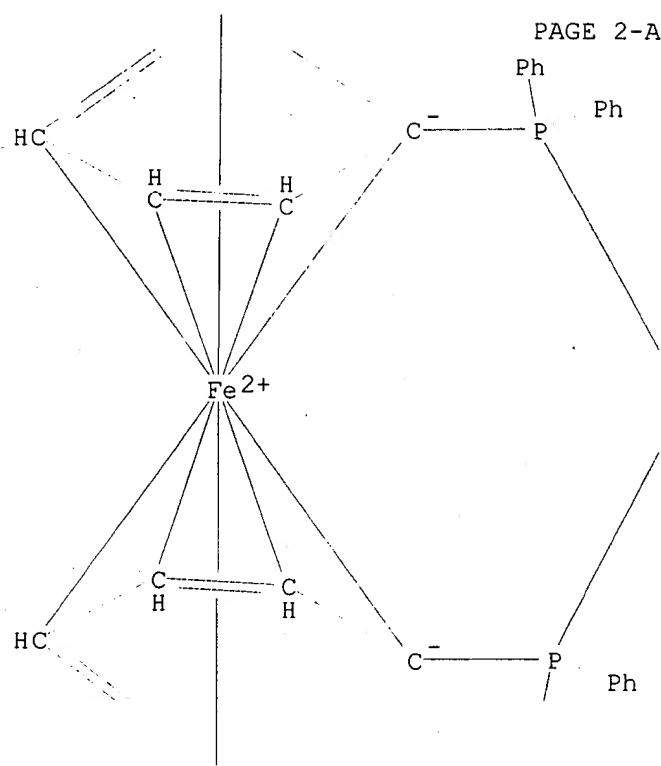
RN 84680-96-6 HCAPLUS

CN Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-
bis(diphenylphosphino-κP)ferrocene]-, perchlorate (9CI) (CA INDEX
NAME)

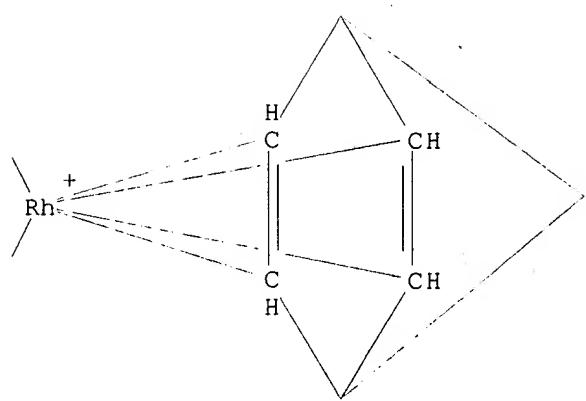
CM 1

CRN 79790-97-9
CMF C41 H36 Fe P2 Rh
CCI CCS

PAGE 2-A

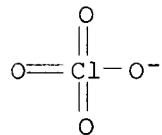


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PAGE 3-A
PhC
H

CM 2

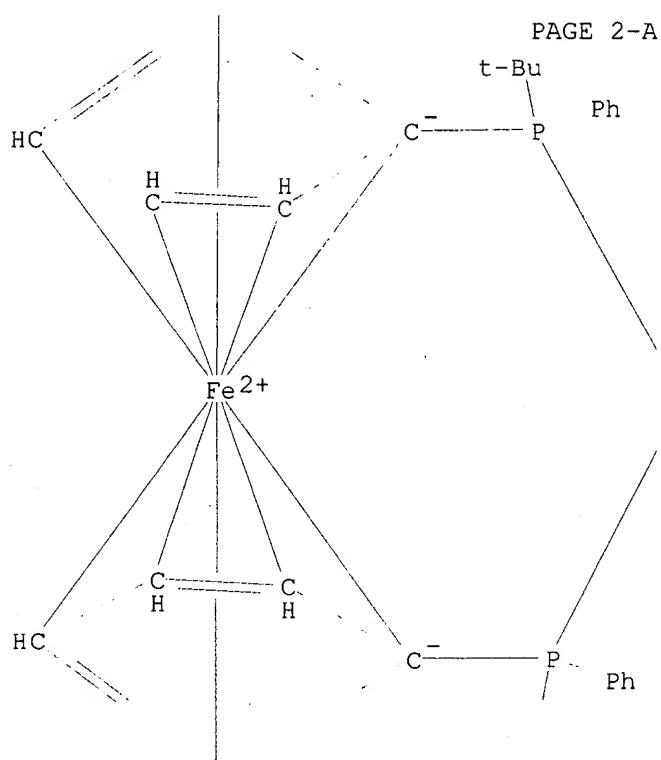
CRN 14797-73-0
CMF Cl O4

RN 92269-95-9 HCAPLUS
CN Rhodium(1+), [(2,3,5,6- η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis[(1,1-dimethylethyl)phenylphosphino]ferrocene-P,P']-, stereoisomer, perchlorate (9CI) (CA INDEX NAME)

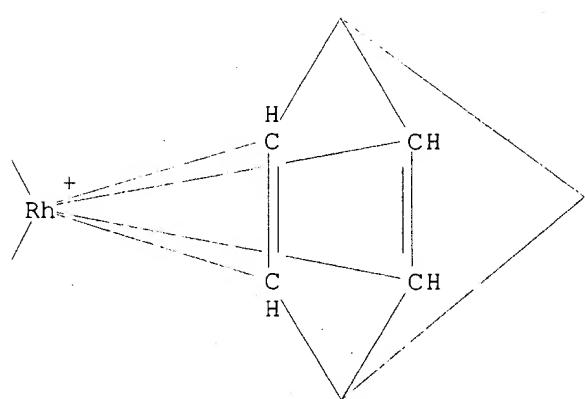
CM 1

CRN 92269-94-8
CMF C37 H44 Fe P2 Rh
CCI CCS

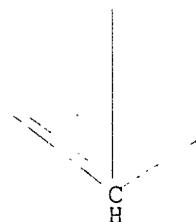
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *



PAGE 2-B

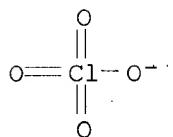


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t-Bu



CM 2

CRN 14797-73-0
CMF C1 O4



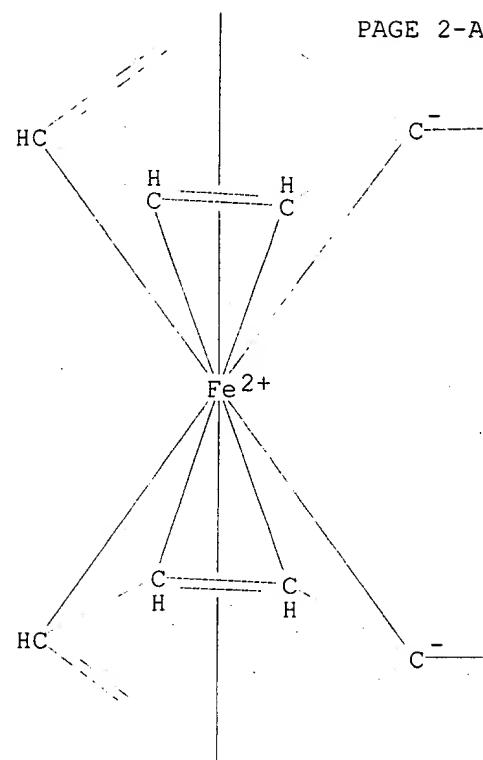
RN 92284-07-6 HCAPLUS
CN Rhodium(1+), [(2,3,5,6- η)-bicyclo[2.2.1]hepta-2,5-diene][1-[bis(1,1-dimethylethyl)phosphino]-1'-(diphenylphosphino)ferrocene-P,P']-, perchlorate (9CI) (CA INDEX NAME)

CM 1

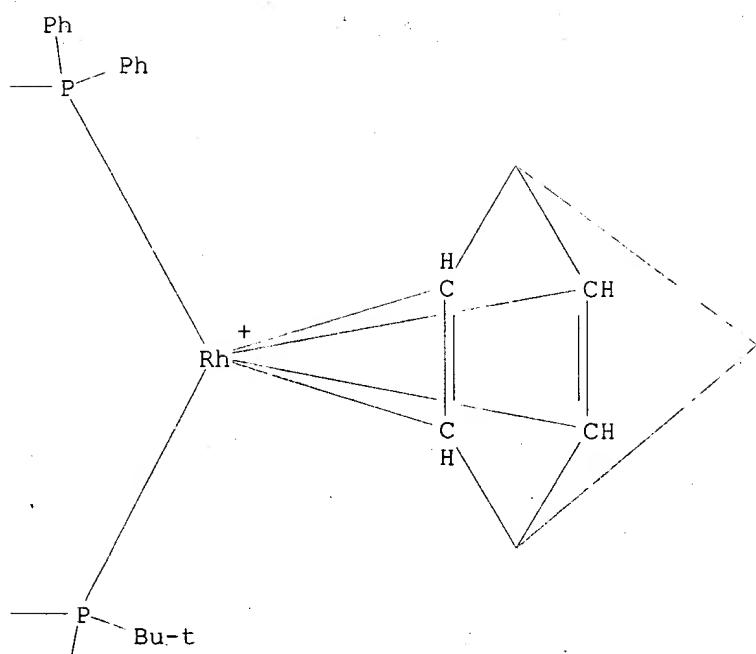
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CMF C37 H44 Fe P2 Rh
CCI CCS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

PAGE 2-A



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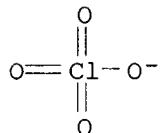
PAGE 3-A

C
H

PAGE 3-B

t-Bu

CM 2

CRN 14797-73-0
CMF Cl O4

IT 84680-98-8

RL: CAT (Catalyst use); USES (Uses)
(catalyst, for **hydrogenation** of alkenes, mol. structure in
relation to kinetics and mechanism with)

RN 84680-98-8 HCAPLUS

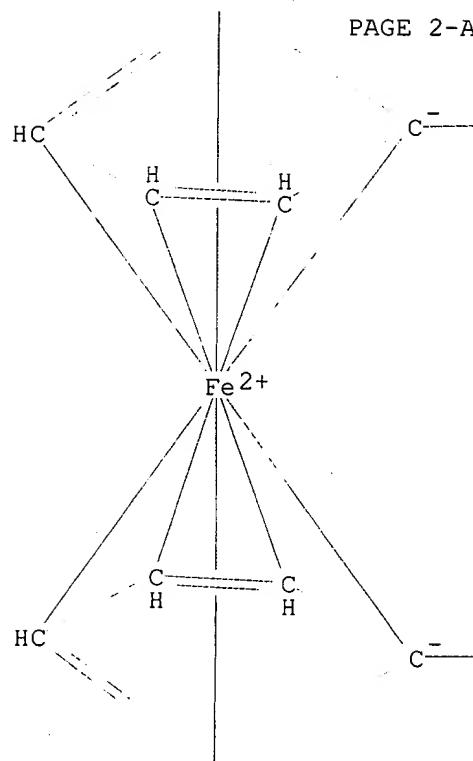
CN Rhodium(1+), [(2,3,5,6- η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-
bis[bis(1,1-dimethylethyl)phosphino]ferrocene-P,P']-, perchlorate (9CI)
(CA INDEX NAME)

CM 1

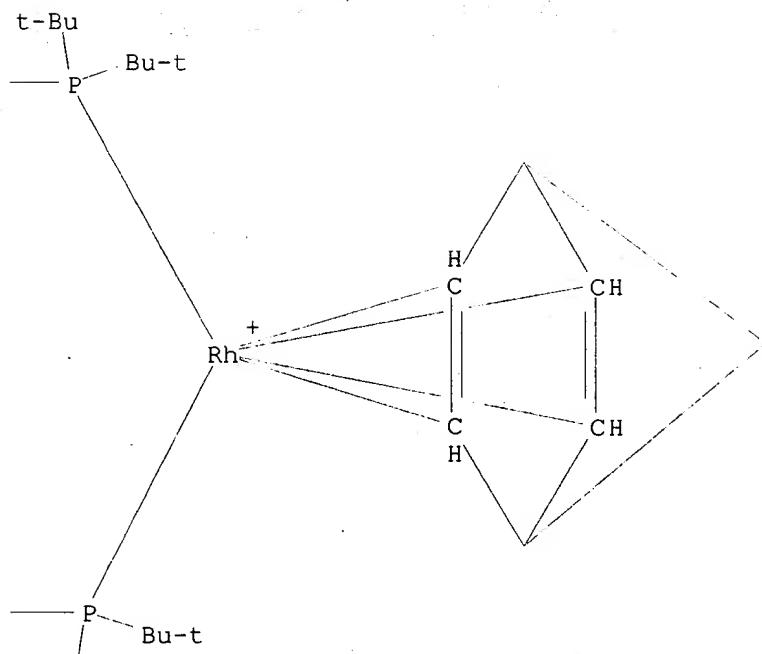
CRN 84680-97-7
CMF C33 H52 Fe P2 Rh
CCI CCS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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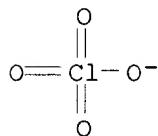
PAGE 3-A

C
H

PAGE 3-B

t-Bu

CM 2

CRN 14797-73-0
CMF Cl O4

L104 ANSWER 18 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN
 AN 1984:571461 HCAPLUS
 DN 101:171461
 ED Entered STN: 10 Nov 1984
 TI Metal hydrides from cationic **rhodium(I)** catalyst precursors.
 X-ray structure of $[(\text{L-L})\text{HRh}(\mu-\text{H})\text{3RhH}(\text{L-L})]\text{ClO}_4$ [$\text{L-L} = \text{rac-Fe}(\eta^5\text{-C}_5\text{H}_4\text{PPhCMe}_3)_2$]
 AU Butler, Ian R.; Cullen, William R.; Kim, Tae Jeong; Einstein, Frederick W.
 B.; Jones, Terry
 CS Chem. Dep., Univ. British Columbia, Vancouver, V6T 1Y6, Can.
 SO Journal of the Chemical Society, Chemical Communications (1984),
 (11), 719-21
 CODEN: JCCCAT; ISSN: 0022-4936
 DT Journal
 LA English
 CC 29-13 (Organometallic and Organometalloidal Compounds)
 Section cross-reference(s): 67, 75
 AB Treatment of $[\text{LRhL1}]\text{ClO}_4$ [$\text{L} = \text{rac-Fe}(\eta^5\text{-C}_5\text{H}_4\text{PPhCMe}_3)_2$,
 $\text{Fe}[\eta^5\text{-C}_5\text{H}_4\text{P}(\text{CMe}_3)_2]_2$ (C_5H_5 = cyclopentadienyl), $\text{L1} = \text{norbornadiene}$]
 with H in MeOH at 30° and 1 atm gave $[\text{LHRh}(\mu-\text{H})\text{3RhLH}]\text{ClO}_4$ (L as
 before) (II and III, resp.). The structures of II and III were determined by
 x-ray anal.
 ST **rhodium ferrocenylphosphine hydride** crystal structure; catalyst
rhodium ferrocenylphosphine hydrogenation
 IT Crystal structure
 Molecular structure
 (of hydride-bridged **rhodium ferrocenylphosphines**)
 IT 84680-98-8 92269-95-9
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (hydrogenation of)

IT 92468-68-3P 92468-70-7P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal and mol. structure of)

IT 92468-67-2P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and mol. structure of)

IT 84680-98-8 92269-95-9

RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrogenation of)

RN 84680-98-8 HCPLUS

CN Rhodium(1+), [(2,3,5,6- η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis[bis(1,1-dimethylethyl)phosphino]ferrocene-P,P']-, perchlorate (9CI)
(CA INDEX NAME)

CM 1

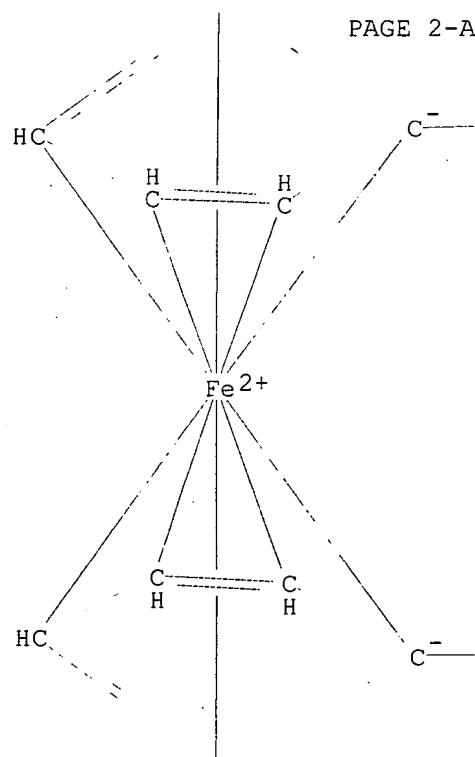
CRN 84680-97-7

CMF C33 H52 Fe P2 Rh

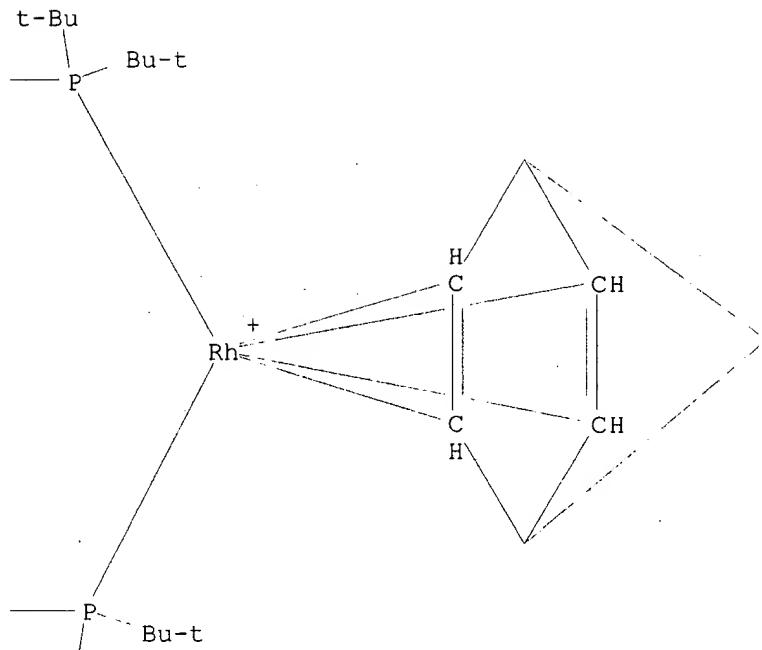
CCI CCS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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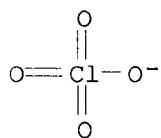
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t-Bu

CM 2

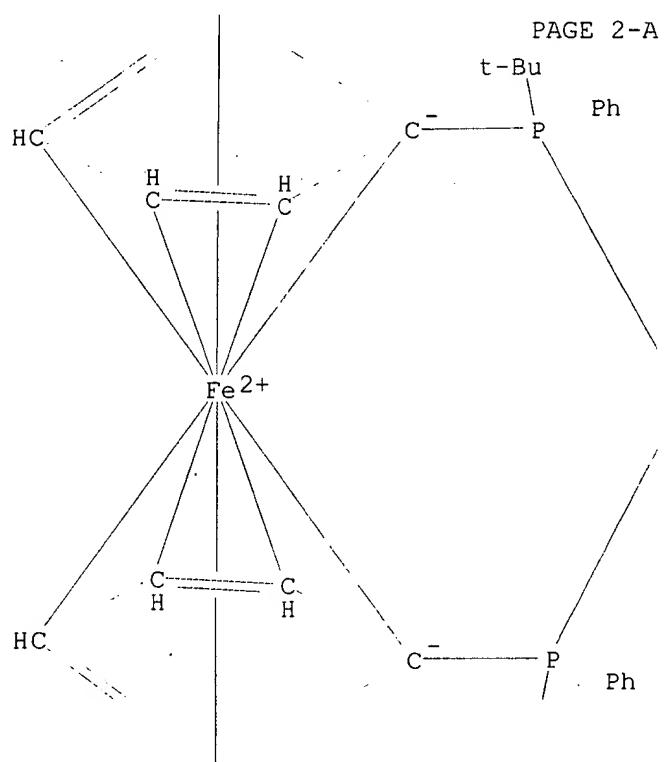
CRN 14797-73-0
CMF Cl O4RN 92269-95-9 HCAPLUS
CN Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis[(1,1-

dimethylethyl)phenylphosphino]ferrocene-P,P']-, stereoisomer, perchlorate
(9CI) (CA INDEX NAME)

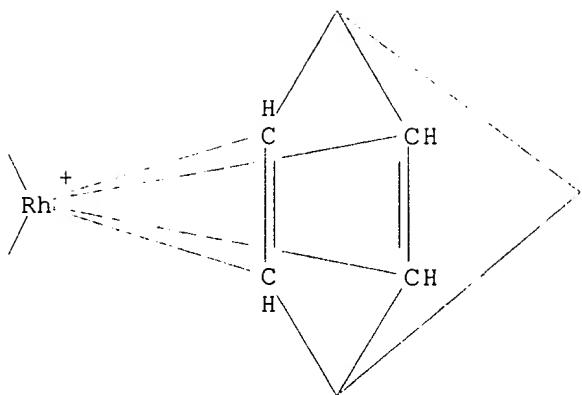
CM 1

CRN 92269-94-8
CMF C37 H44 Fe P2 Rh
CCI CCS

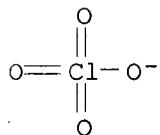
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *



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t-Bu

CM 2

CRN 14797-73-0
CMF Cl 04

IT 92468-68-3P 92468-70-7P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal and mol. structure of)

RN 92468-68-3 HCAPLUS

CN Rhodium(1+), bis[1,1'-bis[(1,1-dimethylethyl)phenylphosphino]ferrocene-
P,P']tri- μ -hydrodihydrodi-, stereoisomer, perchlorate, compd. with
methanol (1:1) (9CI) (CA INDEX NAME)

CM 1

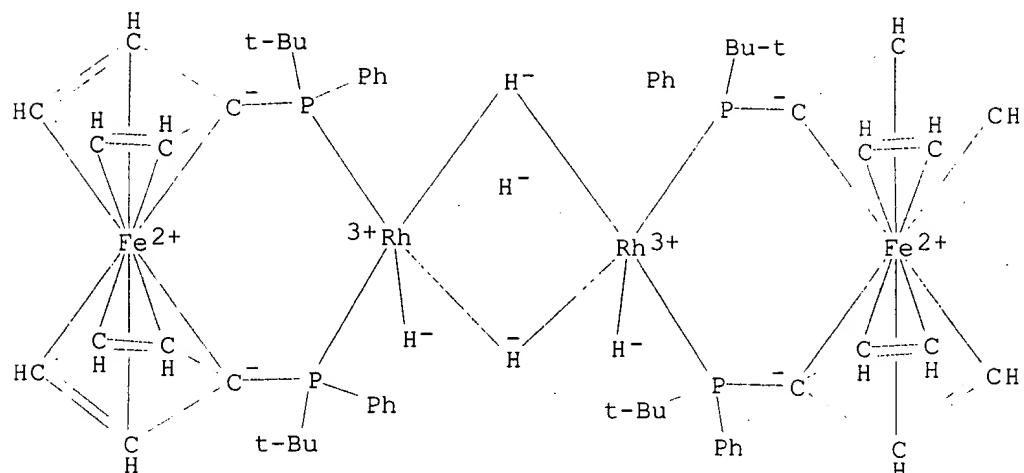
CRN 67-56-1
CMF C H4 O

H₃C--OH

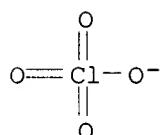
CM 2

CRN 92468-67-2
CMF C60 H77 Fe2 P4 Rh2 Cl O4

CM 3

CRN 92468-66-1
CMF C60 H77 Fe2 P4 Rh2
CCI CCS

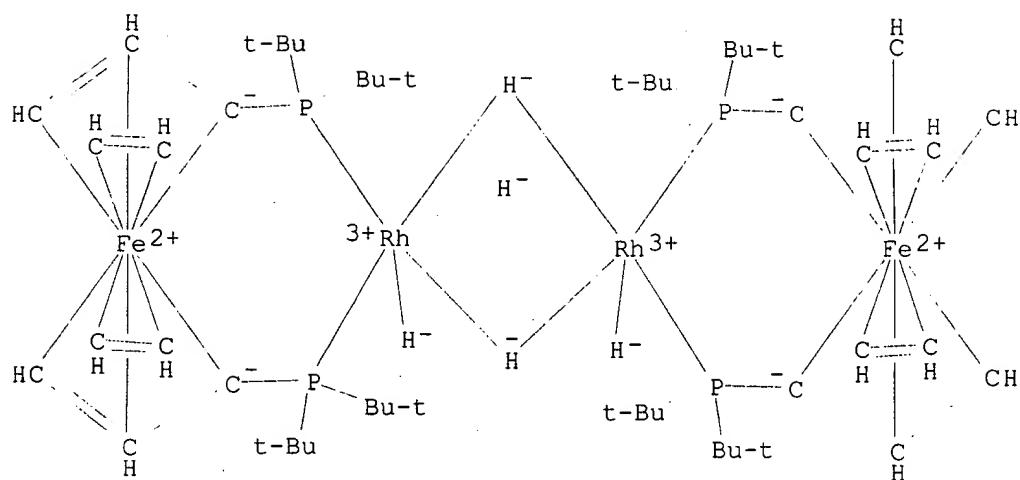
CM 4

CRN 14797-73-0
CMF Cl O4

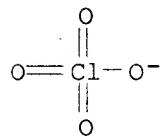
RN 92468-70-7 HCPLUS
 CN Rhodium(1+), bis[1,1'-bis[bis(1,1-dimethylethyl)phosphino]ferrocene-P,P']tri-μ-hydrodihydrodi-, perchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 92468-69-4
CMF C52 H93 Fe2 P4 Rh2
CCI CCS



CM 2

CRN 14797-73-0
CMF C1 O4

IT 92468-67-2P

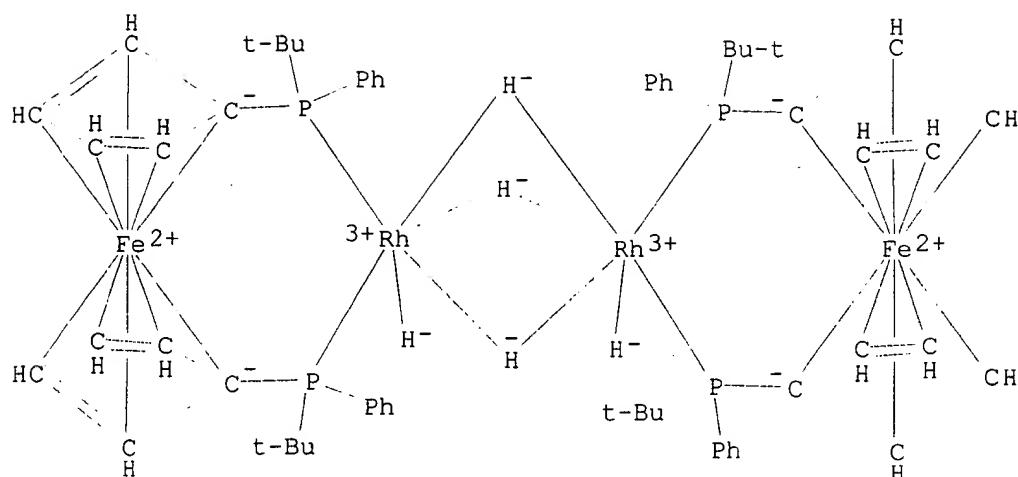
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and mol. structure of)

RN 92468-67-2 HCAPLUS

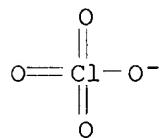
CN Rhodium(1+), bis[1,1'-bis[(1,1-dimethylethyl)phenylphosphino]ferrocene}-P,P']tri- μ -hydrodihydrodi-, stereoisomer, perchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 92468-66-1
CMF C60 H77 Fe2 P4 Rh2
CCI CCS



CM 2

CRN 14797-73-0
CMF Cl O4

L104 ANSWER 19 OF 20 HCPLUS COPYRIGHT 2004 ACS on STN
 AN 1983:215759 HCPLUS
 DN 98:215759
 ED Entered STN: 12 May 1984
 TI Structure of the **hydrogenation** catalyst $[(\text{PP})\text{Rh}(\text{NBD})]\text{ClO}_4$, $\text{PP} = (\eta^5-(\text{Me}_3\text{C})_2\text{PC}_5\text{H}_4)_2\text{Fe}$, and some comparative rate studies
 AU Cullen, William R.; Kim, Tae Jeong; Einstein, Frederick W. B.; Jones, Terry
 CS Chem. Dep., Univ. British Columbia, Vancouver, BC, V6T 1Y6, Can.
 SO Organometallics (1983), 2(6), 714-19
 CODEN: ORGND7; ISSN: 0276-7333
 DT Journal
 LA English
 CC 29-13 (Organometallic and Organometalloidal Compounds)
 Section cross-reference(s): 22, 34, 75
 GI For diagram(s), see printed CA Issue.
 AB In this abstract NBD is norbornadiene. The structure of the homogeneous **hydrogenation** precursor I ($\text{R} = \text{Me}_3\text{C}$).cntdot.**Rh** ($\text{NBD})\text{ClO}_4$ (II), determined crystallog., shows that **Rh** is in a distorted square planar environment involving both NBD double bonds; the bidentate atoms also chelate the **Rh** atom. The steric and electronic effects of the bis(phosphine) ligands in the ferrocenyl moiety are related to the relative **hydrogenation** kinetics of $\text{CH}_2:\text{CRCO}_2\text{H}$ ($\text{R} = \text{NHAc, CH}_2\text{CO}_2\text{H}$) or $\text{PhCH}:\text{CRCO}_2\text{H}$ ($\text{R} = \text{NHAc, Me}$) in EtOH or MeOH containing II or I ($\text{R} = \text{Ph}$).cntdot.**Rh**(NBD) ClO_4 . The mechanism was discussed.
 ST crystal structure **rhodium phosphinoferrocene complex; mol**

structure **rhodium** norbornadiene complex; **hydrogenation**
 catalyst **rhodium** complex; kinetics **hydrogenation**
 acetamidoacrylic acid; mechanism hydration catalyst acetamidoacrylic acid;
 acetamidocinnamic acid kinetics **hydrogenation**; itaconic acid
 kinetics **hydrogenation**; steric effect kinetics
hydrogenation; solvent kinetics **hydrogenation**

IT Ligands
 RL: RCT (Reactant); RACT (Reactant or reagent).
 (bis(phosphino)ferrocenes, for **rhodium** in homogeneous
hydrogenation catalyst, substituent effects and)

IT Bond
 (in **rhodium** complex homogeneous **hydrogenation**
 catalyst containing bis(phosphino)ferrocene ligands)

IT Kinetics of **hydrogenation**
 (of alkenoic acids in presence of **rhodium** complexes containing
 bis(phosphino)ferrocenes)

IT **Hydrogenation**
 (of alkenoic acids, in presence of **rhodium** complexes containing
 bis(phosphino)ferrocenes, mechanism of)

IT Crystal structure
 Molecular structure
 (of **rhodium** complex with bis(phosphino)ferrocene)

IT Steric effect
 Substituent effect
 (on **hydrogenation** activity of **rhodium** complexes
 containing bis(phosphino)ferrocenes)

IT Solvent effect
 (on **hydrogenation** of alkenoic acids in presence of
rhodium complexes with bis(phosphino)ferrocenes)

IT **Hydrogenation catalysts**
 (**rhodium** complexes containing norbornadiene and
 bis(phosphino)ferrocenes, for alkenoic acids, kinetics and mechanism
 with)

IT Carboxylic acids, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (unsatd., **hydrogenation** of, in presence of **rhodium**
 complexes containing bis(phosphino)ferrocenes)

IT 84680-96-6 84680-98-8
 RL: CAT (Catalyst use); USES (Uses)
 (**hydrogenation** catalyst, for alkenoic acids, kinetics and
 mechanism with)

IT 97-65-4, reactions 1199-77-5 5429-56-1 5469-45-4
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (**hydrogenation** of, in presence of **rhodium** complexes
 with norbornadiene and bis(phosphino)ferrocenes, kinetics and mechanism
 of)

IT 84680-95-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and complexation of, with **rhodium** and norbornadiene)

IT 11106-52-8
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with chlorodibutylphosphine)

IT 13716-10-4
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with dilithioferrocenebis(tetramethylethylenediamine))

IT 84680-96-6 84680-98-8
 RL: CAT (Catalyst use); USES (Uses)
 (**hydrogenation** catalyst, for alkenoic acids, kinetics and
 mechanism with)

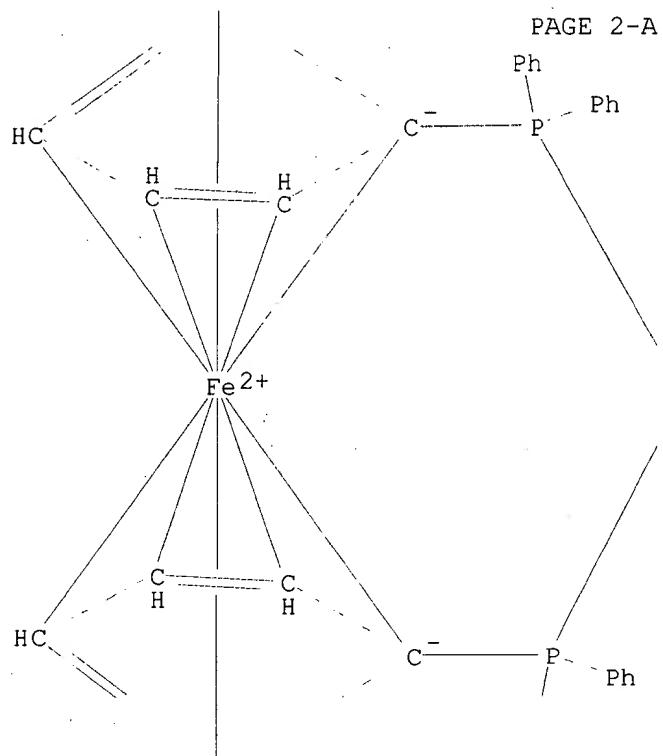
RN 84680-96-6 HCPLUS

CN Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-
 bis(diphenylphosphino-κP)ferrocene]-, perchlorate (9CI) (CA INDEX
 NAME)

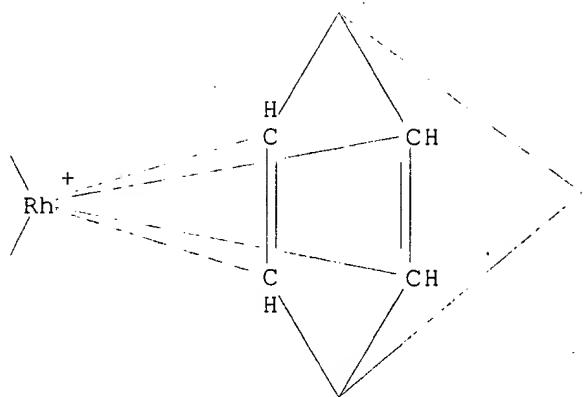
CM 1

CRN 79790-97-9
CMF C41 H36 Fe P2 Rh
CCI CCS

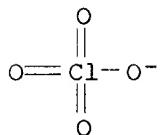
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *



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PAGE 3-A
Ph

CM 2

CRN 14797-73-0
CMF Cl O4

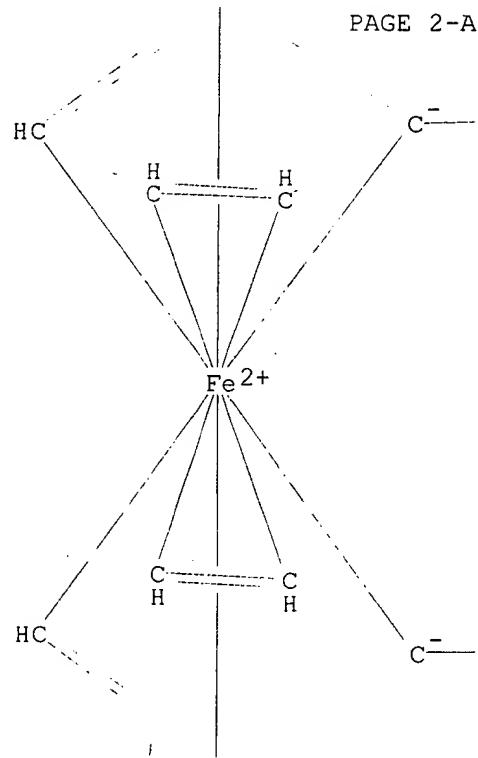
RN 84680-98-8 HCAPLUS
 CN Rhodium(1+), [(2,3,5,6- η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis[bis(1,1-dimethylethyl)phosphino]ferrocene-P,P']-, perchlorate (9CI)
 (CA INDEX NAME)

CM 1

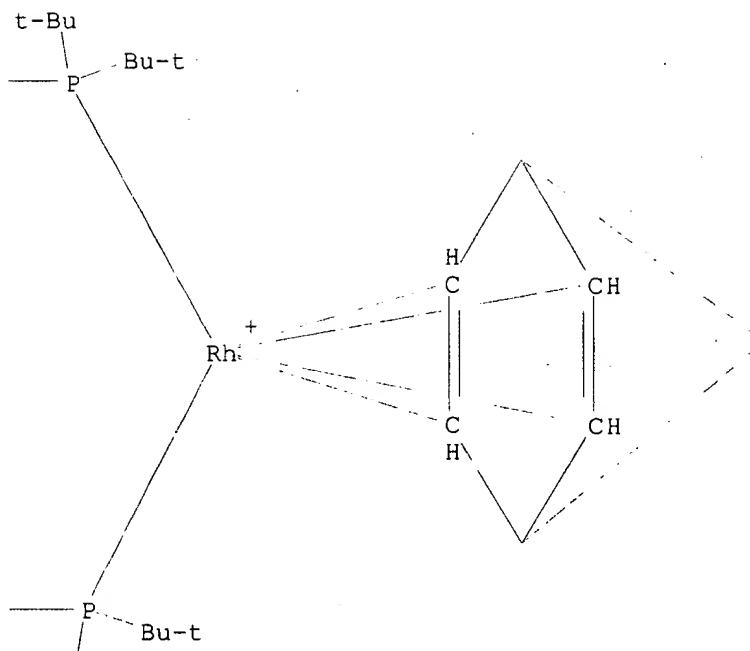
CRN 84680-97-7
CMF C33 H52 Fe P2 Rh
CCI CCS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

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PAGE 3-A

C
H

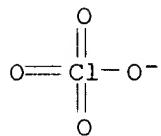
PAGE 3-B

t-Bu

CM 2

CRN 14797-73-0

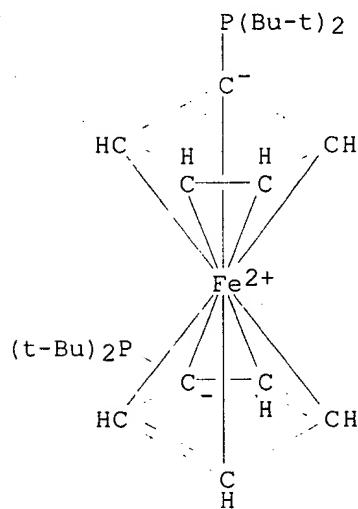
CMF Cl O4



IT 84680-95-5P

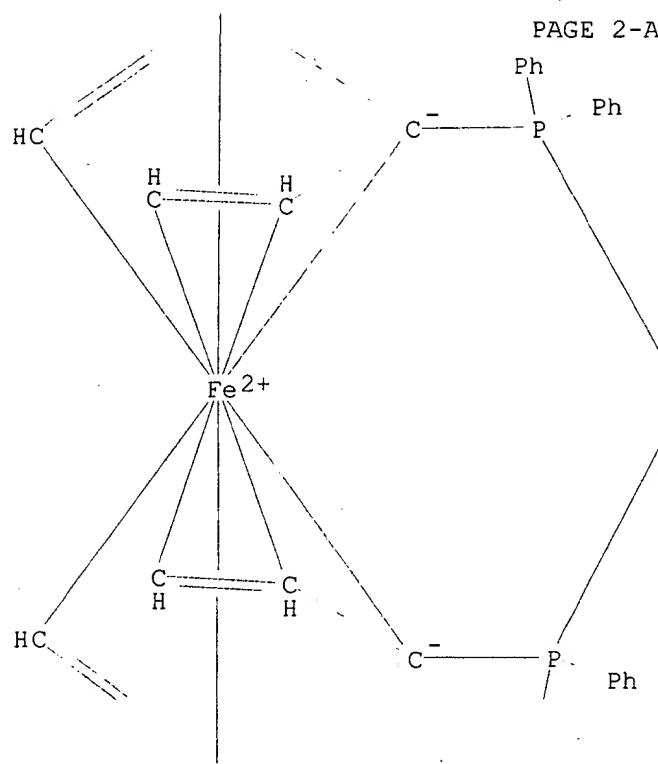
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and complexation of, with rhodium and norbornadiene)

RN 84680-95-5 HCAPLUS

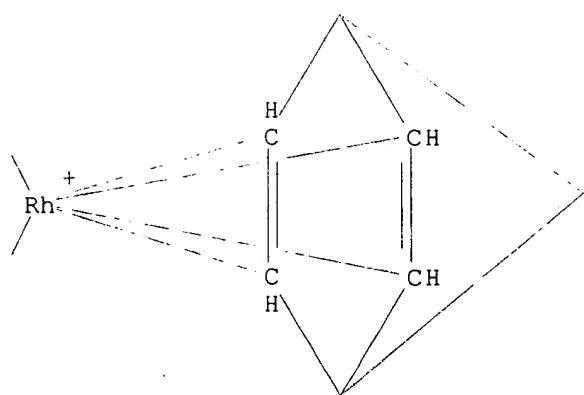
CN Ferrocene, 1,1'-bis[bis(1,1-dimethylethyl)phosphino]- (9CI) (CA INDEX
NAME)

DN 95:210374
 ED Entered STN: 12 May 1984
 TI The mechanism of asymmetric homogeneous hydrogenation. Solvent complexes and dihydrides from rhodium diphosphine precursors
 AU Brown, John M.; Chaloner, Penny A.; Kent, Alexander G.; Murrer, Barry A.; Nicholson, Philip N.; Parker, David; Sidebottom, Philip J.
 CS Dyson Perrins Lab., Oxford, OX1 3QY, UK
 SO Journal of Organometallic Chemistry (1981), 216(2), 263-76
 CODEN: JORCAI; ISSN: 0022-328X
 DT Journal
 LA English
 CC 67-1 (Catalysis and Reaction Kinetics)
 Section cross-reference(s): 22
 AB Bicyclo[2.2.1]hepta-2,5-diene and cycloocta-1,5 diene(biphosphine)Rh tetrafluoroborates react with H at 1 atm in methanol or other polar solvents to give as initial product either a solvated dihydride or a solvate. Depending on phosphine structure the equilibrium between these 2 species varies widely. Dihydrides are normally the stable product when the ligand is a monophosphine although (o-methoxyphenyl)methylphenylphosphine is an exception. Cis Chelating biphosphines normally form solvate complexes with no affinity for H. R-Ph bis(diphenylphosphinoethane) falls into this category, but the 31P NMR spectra of its complexes demonstrate an equilibrium between monomeric and dimeric species, and addition of triethylamine gives rise to a trimer. Trans-Chelating biphosphines show more variable behavior, and in the case of bis-1,5-diphenylphosphinopentane, a number of complexes, including one requiring C-H activation, were observed
 ST hydrogenation catalyst rhodium phosphine olefin; bicycloheptadiene rhodium phosphine hydrogenation catalyst; cyclooctadiene rhodium phosphine hydrogenation catalyst
 IT Hydrogenation catalysts
 (rhodium bicycloheptadiene by phosphinetetrafluoroborates, solvent complexes and dihydrides of)
 IT 79790-95-7
 RL: CAT (Catalyst use); USES (Uses)
 (hydrogenation catalysts, preparation of solvent complexes and dihydrides of)
 IT 34664-30-7 34664-31-8 60430-43-5 60584-05-6 65606-90-8
 68811-61-0 68811-82-5 74498-00-3 75085-38-0 79255-71-3
 79790-89-9 79790-91-3 79790-98-0 79795-96-3
 RL: CAT (Catalyst use); USES (Uses)
 (hydrogenation catalysts, solvent complexes and dihydrides of)
 IT 69381-91-5P 121902-83-8P
 RL: PREP (Preparation)
 (preparation of)
 IT 79790-98-0
 RL: CAT (Catalyst use); USES (Uses)
 (hydrogenation catalysts, solvent complexes and dihydrides of)
 RN 79790-98-0 HCPLUS
 CN Rhodium(1+), [(2,3,5,6- η)-bicyclo[2.2.1]hepta-2,5-diene][1,1'-bis(diphenylphosphino- κ P)ferrocene]-, tetrafluoroborate(1-) (9CI)
 (CA INDEX NAME)
 CM 1
 CRN 79790-97-9
 CMF C41 H36 Fe P2 Rh
 CCI CCS

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PAGE 2-B

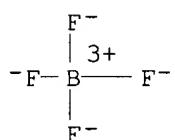


PAGE 3-A
Ph

C
H

CM 2

CRN 14874-70-5
CMF B F4
CCI CCS



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